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CITPUFF: A Gaussian Puff Model for Estimating Pollutant Concentration in Complex Terrain

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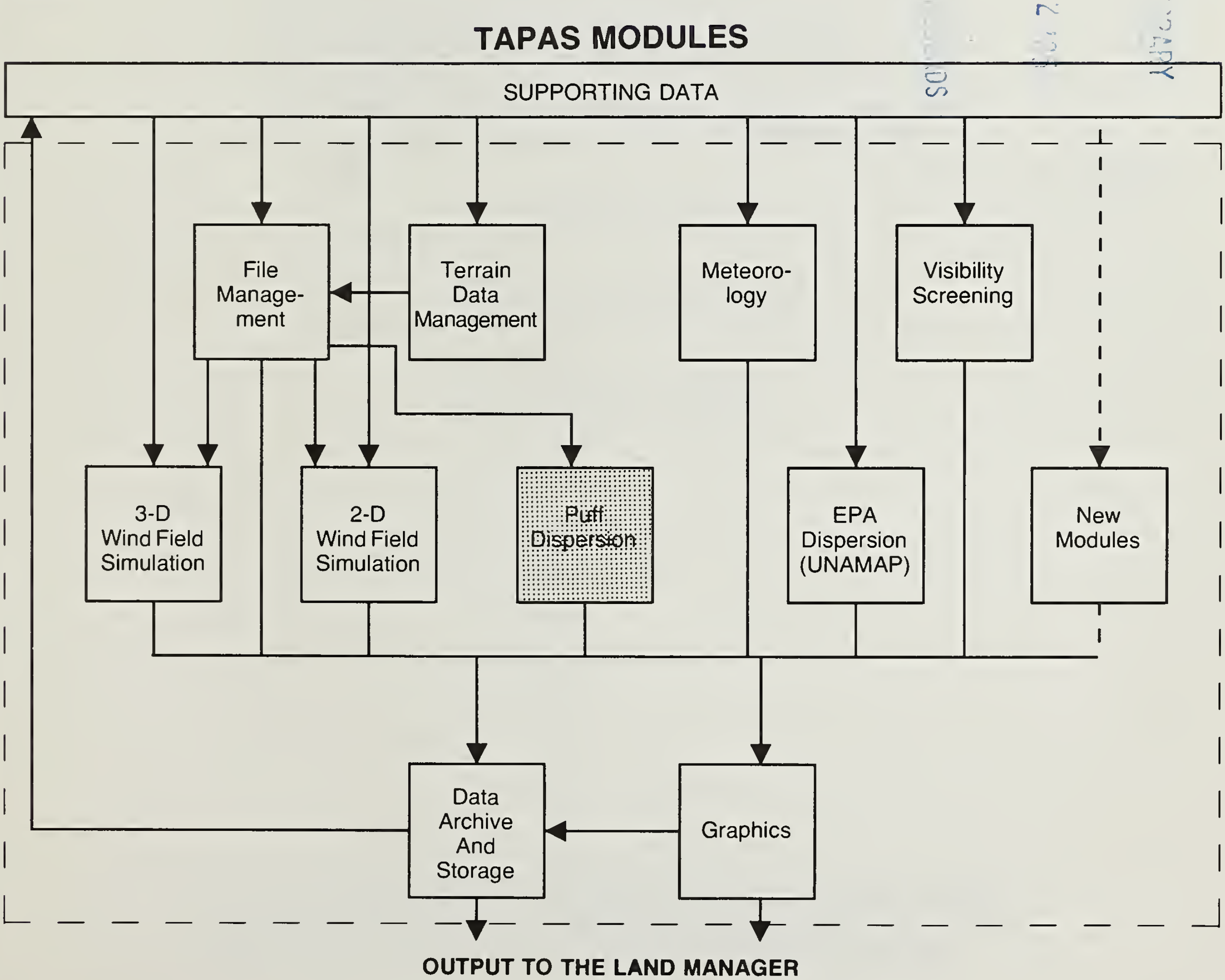

Abstract

CITPUFF, is a puff-type dispersion model that uses a wind field calculated from a complex-terrain wind model. It accommodates a variety of source types including point, area, and line sources; calculates plume rise where applicable; and outputs a graphic display of puff trajectories and concentrations. The model is compared against models currently used for assessing air quality impacts in complex topography.

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CITPUFF: A Gaussian Puff Model for Estimating Pollutant Concentration in Complex Terrain[1]

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MANAGEMENT IMPLICATIONS

This paper presents technical details of an air pollution dispersion model implemented as a component of the Topographic Air Pollution Analysis System (TAPAS). TAPAS is a user-friendly, semi-interactive, collection of computer programs implemented on the Colorado State University CDC-Cyber computer. The programs are written in CDC's version of FORTRAN IV.

TAPAS includes a number of programs that fit into three categories: file management routines, models, or input/output routines. File management routines allow the user to construct data files, model submit files, and output submit files. The input/output routines allow the user to access data and to output graphic products to various graphics-capable hardware. The models, however, represent the central value of TAPAS. They are designed to simulate air flow in mountainous terrain and the dispersion of pollution released from various sources in mountainous terrain. A primary objective of TAPAS is to increase the utility of such models by including them in a user-oriented environment. A second objective is to provide as wide an array of models as possible. This is important because mountain air quality and related air resource problems are very complex. It is unlikely that any one approach, technique, or model will be adequate for all purposes. Furthermore, sufficient data resources do not exist to establish overall validity of alternative techniques. TAPAS provides a range of techniques in a friendly environment so that the user can select the most appropriate technique for a particular application.

The CITPUFF model described in this paper is a dispersion model; together with the WINDS model, it provides an approximation of the physical situation which may be helpful in conducting certain types of planning analyses. It is a reasonably economical system. Should the user interest be in more specific real-time or operations-oriented modeling, the approach here may be useful but great caution is appropriate. The last section of this report describes the limitations in the model physics, which are significant, and highlights what may be appropriate applications.

INTRODUCTION

Predicting the concentration of air pollutants is a problem that increases in significance with industrial development and population increases. In mountainous areas, particularly in the western United States, development is generally associated with mineral production and recreational opportunities. The Clean Air Act requires significant involvement for federal land managers in the review of prevention of significant deterioration (PSD) permits (Part C, Public Law 95-95). In addition, federal land managers are responsible for managing pollution their activities generate, like smoke from prescribed burning. For both of these air quality models capable of predicting the concentration of pollution that would result from a source in mountainous terrain are needed. A gaussian puff model, the Complex Interactions with Terrain-Puff Model (CITPUFF), was designed to partially meet this need.

To predict concentrations in complex topography, it is necessary to estimate (1) the meteorology of the region in some detail; (2) the diffusion of pollution; and (3) the removal and/or chemical transformation of pollutants. To support these estimates, the Topographic Air Pollution Analysis System (TAPAS) has been developed (Fox and Fosberg 1977, Childs and Marlatt 1981, Fox et al. 1984). TAPAS includes a series of air quality related models and procedures. Because applications are anticipated in data-poor areas, wind models are among the most significant elements of TAPAS. WINDS (Fosberg et al. 1976) is a TAPAS model that is capable of providing a grid-based, diagnostic, two-dimensional distribution of wind speed and direction. WINDS provides an analysis of the distribution of winds in complex terrain based on an assumed (or measured) primary influencing wind. The WINDS model generated wind field can be used as the basis for estimating plume trajectories in the pollution transport and dispersion modules of TAPAS. This document describes the primary TAPAS pollution transport and dispersion module, CITPUFF.

CITPUFF is a Lagrangian "puff-type" diffusion model based on the Start and Wendell (1974) model, MESODIF (also Bass et al. 1979). Pollution released from a source is transported by the wind while it diffuses as a result of the atmospheric turbulence. The details of the source must be described in terms of the source location, type of pollution, rate of emission, and the physical source parameters (point source, area source, height of stacks, etc.). CITPUFF calculates the appropriate plume rise using EPA-recommended procedures (EPA 1978, 1980). An initial source dispersion parameter is used as an option to accommodate a number of different source types, ranging from an isolated point source, to a time-dependent forest burn, to an area source such as a surface mine. The puff is diffused according to conventional theories of atmospheric turbulence. Empirical classes of atmospheric stability used in the model are related to the level of atmospheric turbulence. The user may select from three options for dispersion, including a fixed 22.5° horizontal spread, standard Pasquill-Gifford-Turner disper-

sion coefficients, and a convective boundary layer based scheme using altered Pasquill-Gifford coefficients. The CITPUFF model also allows a linear depletion of mass from the puff. Puffs are released at a user-selected rate and tracked until they are transported off the wind field grid. Concentration is accumulated at receptors located at each computational grid point to determine the ground-level concentration of pollutants.

First, the document describes the general theory on which CITPUFF is based. Then it develops the details of CITPUFF, including the grid system, meteorology, emissions configurations, terrain height adjustment, diffusion coefficients, mixing depth adjustments, and puff sampling functions. The last section identifies how CITPUFF performs relative to other models and modeling techniques and discusses appropriate limitations on model use.

CITPUFF MODEL—GENERAL THEORY

When the principle of conservation of mass is applied in the atmosphere, together with a Fickian approximation for molecular diffusion, it yields the following form of the diffusion equation:

$$\frac{\partial \chi}{\partial t} + \nabla(\chi \mathbf{V}) = \nabla(D\nabla\chi) + \Sigma S \qquad [1]$$

where

$\chi(\mathbf{x},t)$ = instantaneous, realized concentration at time t at position x relative to a given origin,
$\mathbf{x} = (x,y,z)$ = Cartesian coordinates,
$\mathbf{V}$ = velocity field,
D = molecular diffusivity,
ΣS = sum of sources and sinks.

In the present case, ΣS is replaced by the term $-k\chi$ which may be used to account for such nonconservative effects as first-order removal, conversion of gaseous to particulate pollutants, and radioactive decay. In such cases the rate of loss of the diffusing material is assumed proportional to its concentration, the factor of proportionality, k, being a "decay constant" of dimensions s^{-1}.

In turbulent flow both fluid velocity and tracer concentration are random variables. These variables may be separated into ensemble mean and fluctuating components. To focus attention on the effects of complex topography on dispersion, the approach of Fosberg and Fox (1978) is extended and the fluctuating components are considered to be composed of topographically induced effects and the usual flat-terrain turbulent fluctuation, as follows:

$$\mathbf{V} = \bar{\mathbf{V}} + \hat{\mathbf{V}} + \mathbf{V}'$$

$$\chi = \bar{\chi} + \hat{\chi} + \chi'$$

where

$\bar{\mathbf{V}},\bar{\chi}$ = ensemble mean values,

$\hat{\mathbf{V}},\hat{\chi}$ = terrain-induced fluctuations about the mean,

$\mathbf{V}',\chi'$ = the remaining small-scale variations from the ensemble mean, generally considered as flat-terrain turbulent fluctuations.

Taking ensemble averages of both sides of equation [1] yields

$$\frac{\partial \bar{\chi}}{\partial t} + \nabla(\bar{\chi}\bar{\mathbf{V}}) + \nabla(\hat{\chi}\hat{\mathbf{V}}) + \nabla(\chi'\mathbf{V}') = \nabla(D\nabla\bar{\chi}) - k\bar{\chi} \qquad [2]$$

The velocity-concentration correlation $\bar{\chi}'\bar{\mathbf{V}}'$ represents flux by turbulent movements and can be related to mean flow variables with a Fickian diffusion approximation. Eddy diffusivities, $\mathbf{K} = (K_x, K_y, K_z)$, can be substituted into equation [2]

$$\frac{\partial \bar{\chi}}{\partial t} + \bar{\mathbf{V}}\nabla\bar{\chi} = \nabla(\mathbf{K}\nabla\bar{\chi}) - k\bar{\chi} - \nabla(\bar{\hat{\chi}}\bar{\hat{\mathbf{V}}}) \qquad [3]$$

where molecular diffusion has been neglected relative to turbulent diffusion, and the second term on the left-hand side of equation [2] has been simplified by using the ensemble mean form of the continuity equation for an incompressible fluid ($\nabla\bar{\mathbf{V}} = 0$).

The concentration-velocity correlation, $\hat{\chi}\hat{\mathbf{V}}$, represents flux by terrain-induced motion. In order to "directly" close equation [3] one can postulate a Fickian-type diffusion approximation to relate $\hat{\chi}\,\hat{\mathbf{V}}$ mean flow variables, with Cartesian components of the form:

$$\hat{\chi}\hat{u} = -C_x \frac{\partial \bar{\chi}}{\partial x}, \quad \hat{\chi}\hat{v} = -C_y \frac{\partial \bar{\chi}}{\partial y}, \quad \hat{\chi}\hat{w} = -C_z \frac{\partial \bar{\chi}}{\partial z}$$

The terrain-induced "apparent diffusivities" (C_x, C_y, C_z) will depend both on nonturbulent, organized, circulation patterns induced by the terrain, and on topographically induced turbulent enhancement. In both cases, there will be a direct, or at least implicit, dependence on differential thermal convection from mountain slope surfaces, coupled with mechanical interactions of the terrain with the mean winds.

The nonturbulent component accounts for terrain-induced kinematic constraints of the flow, and their subsequent effects on horizontal and vertical dispersion. These kinematic constraints are produced by distortions caused by air flow around terrain obstacles that produce phases of acceleration and deceleration that can be regarded as independent of turbulent diffusion to the first order.

Terrain-induced kinematic constraints on plume dispersion and plume trajectories have been examined by Hunt and Mulhearn (1973), Egan (1975), and Hunt et al. (1978) using the theory of turbulent plumes embedded within potential flow fields. Bass et al. (1981) extended this approach to slightly stable flows by an empirical ap-

proximation derived from stratified tow-tank experiments (Snyder 1981), as well as for objects of arbitrary crosswind aspect ratio. Bass et al. (1981) present a comprehensive review of the work performed by using this approach, as well as a discussion of the associated limitations. In particular, this report provides a detailed description of the circumstances and limitations associated with a simplistic inclusion of flow fluid distortions on a Gaussian plume model.

Recently, a considerable amount of research has been directed toward understanding the behavior of plumes in simplified topographic settings. Laboratory simulation and actual field studies have been compiled for Cinder Cone Butte in Idaho, a small, Gaussian-shaped, 100-m-high hill. The reports from this study (Lavery et al. 1982, Lavery et al. 1983, Strimaitis et al. 1983) suggest that dispersion coefficients for use in modified Gaussian models should be calculated from measurements of the local turbulence level. This is not a particularly surprising result, and it suggests that emphasis should be placed on proper measurement, or simulation of the wind field and its associated turbulence. These studies have also clearly established the concept of the dividing streamline in stable flows. This is a level in the atmosphere where the kinetic energy an air parcel contains is matched by the potential energy required to lift the parcel against the density gradient. This height, in a simple situation with uniform wind and temperature profiles, is given by

$$h_d = (1 - F_r)h$$

$$F_r = \frac{u}{Nh}$$

$$N = \left(\frac{g}{\theta} \cdot \frac{d\theta}{dz}\right)^{1/2}$$

where

h_d = dividing streamline height,
u = uniform velocity upstream of the hill,
h = height of the topography,
θ = potential temperature,
g = acceleration of gravity.

This height separates two vastly different flow regimes. Above this level, air will flow over the topography; below this level, air essentially stagnates. This research clearly demonstrates the need to make local measurements in complex terrain. It also shows that even simple situations in complex topography lead to remarkable complexity in the flow. As a final objective, this EPA-supported research is expected to yield improved formulations for dispersion coefficients and stability effects in complex topography. In view of this, CITPUFF employs a modular approach allowing the incorporation of new procedures as they become available.

Within the context of a puff model, terrain-induced alterations of the puff/plume centerline can be handled via the wind field input that is used to transport the puff. The effect of terrain on dispersion by kinematic effects and the effects of local turbulence can be incorporated by adjusting the flat-terrain dispersion coefficients. The latter adjustments could perhaps be achieved by postulating relationships between the diffusivities C_x, C_y, and C_z and variables such as streamline convergence and divergence, which characterize phases of acceleration and deceleration. This approach must be merged with an understanding of turbulence generation via these mechanisms and is beyond the scope of this report. Unfortunately, the current state of knowledge in this area (Egan 1984)[4] is inadequate. The current discussion is included simply to illustrate that a theoretical basis and a mechanism for incorporating these effects into a Gaussian-type model by the dispersion relations exist. The discussion that follows, however, will use the flat-terrain dispersion relations and account for terrain effects via the wind field and a terrain height adjustment algorithm because the state of knowledge at present does not support alteration of dispersion coefficients (Strimaitis et al. 1983).

Equation [3] can now be written in the form:

$$\frac{\partial \bar{\chi}}{\partial t} + \bar{u}\frac{\partial \bar{\chi}}{\partial x} = \frac{\partial}{\partial x} K_x'\left(\frac{\partial \bar{\chi}}{\partial x}\right) + \frac{\partial}{\partial y}\left(K_y'\frac{\partial \bar{\chi}}{\partial y}\right) + \frac{\partial}{\partial z}\left(K_z'\frac{\partial \bar{\chi}}{\partial z}\right) - K_x' \qquad [4]$$

where

$$\bar{\mathbf{V}} = (\bar{u},0,0)$$

$$K_x' = K_x + C_x,\ K_y' = K_y + C_y,\ K_z' = K_z + C_z$$

The final term on both sides of equation [4] can be eliminated by the change of variable

$$\bar{c} = \bar{\chi} \exp(-kx/\bar{u}) \exp(x\bar{u}/2K_x') \exp(-\bar{u}^2 t/4K_x')$$

to obtain

$$\frac{\partial \bar{c}}{\partial t} = \frac{\partial}{\partial x} K_x'\left(\frac{\partial \bar{c}}{\partial x}\right) + \frac{\partial}{\partial y}\left(K_y'\frac{\partial \bar{c}}{\partial y}\right) + \frac{\partial}{\partial z}\left(K_z'\frac{\partial \bar{c}}{\partial z}\right) \qquad [5]$$

A solution to equation [5] for an instantaneous point source of strength Q (units of mass), generated at time t = 0 located at the origin of the Cartesian coordinate system was first obtained by Roberts (1923) as

$$\bar{c} = \frac{Q}{(2\pi)^{3/2}\sigma_x\sigma_y\sigma_z} \exp\left[-\left(\frac{x^2}{2\sigma_x^2} + \frac{y^2}{2\sigma_y^2} + \frac{z^2}{2\sigma_z^2}\right)\right] \qquad [6]$$

where it has been assumed that a Gaussian distribution in x, y, and z for the concentration exists, and such a distribution is related to the "eddy" diffusivity (assumed constant) by

$$\begin{aligned} \sigma_x^2 &= 2tK_x' = 2t(K_x + C_x) \\ \sigma_y^2 &= 2tK_y' = 2t(K_y + C_y) \\ \sigma_z^2 &= 2tK_z' = 2t(K_z + C_z) \end{aligned} \qquad [7]$$

[4]*Egan, B. A. 1984. Workshop report on air quality modeling in complex terrain—Keystone, Colorado, May 1983. American Meteorological Society, Boston, Mass. (In press).*

The solution is

$$\bar{\chi}=\frac{Q}{(2\pi)^{3/2}\sigma_x\sigma_y\sigma_z}\exp\left[-\left(\frac{(x-\bar{u}t)^2}{2\sigma_x^2}+\frac{y^2}{2\sigma_y^2}+\frac{z^2}{2\sigma_z^2}\right)\right]\exp(-kx/\bar{u}) \quad [8]$$

for the case of a puff from an instantaneous point source that is advected in the x direction with a mean wind speed $\bar{u}$, while losing mass at an exponential rate k as a result of the assumed first-order decay.

For a puff generated from a point source with an effective emission height h above ground level, equation [8] becomes

$$\bar{\chi}(x,y,z)=\frac{Q}{(2\pi)^{3/2}\sigma_y^2\sigma_z}\exp\left(\frac{-r^2}{2\sigma_y^2}\right)\left\{\exp\left[\frac{-(z-h)^2}{2\sigma_z^2}\right]+\exp\left[\frac{-(z+h)^2}{2\sigma_z^2}\right]\right\}\exp(-kx/\bar{u}) \quad [9]$$

where $r^2=(x-\bar{u}t)^2+y^2$, and where horizontal Gaussian symmetry has been assumed (i.e., $\sigma_x=\sigma_y$). In this form the actual source (with stack height h_s) is located at the point $(0,0,h_s)$. The second term in the large bracket results from an image source (of the effective source) at $(0,0,-h_s)$ to represent the effect of the ground.

The resulting ground-level concentration for a discrete puff, in the form

$$\bar{\chi}(x,y,0)=\frac{2Q}{(2\pi)^{3/2}\sigma_y^2\sigma_z}\exp\left(\frac{-r^2}{2\sigma_y^2}\right)\exp\left(\frac{-h^2}{2\sigma_z^2}\right)\exp\left(\frac{-kx}{\bar{u}}\right) \quad [10]$$

is used as the basic building block for the puff component of the model.

Source emissions are simulated as a time series of discrete puffs. At each time step, the puff centroids are advected by a two-dimensional Lagrangian trajectory function. The standard deviations of the assumed Gaussian concentration distributions are taken to be power law functions of travel distance/time.

The extension to multiple sources is based on the assumption that the total concentration field of a pollutant can be obtained by superposition of the concentration fields for each individual source.

Line, area, and volume source distributions can be simulated by the use of virtual point sources and the specifications of initial values of the Gaussian standard deviations (σ_{yo} and σ_{zo}) characteristic of the particular source distribution. Care must be exercised in modeling cases where these dimensions may vary with temporal or local spatial changes in wind direction and speed. When local spatial changes are evident, it may be necessary to represent a large area source by more than one puff in order to properly represent the flow, since the trajectory function only considers the centroid of each puff.

The CITPUFF model is designed to predict pollutant concentrations at specific receptors. At any such receptor the model calculates the integrated concentration,

$$\psi_s=\int_{t_o}^{t_o+T}\bar{\chi}_s dt \quad [11]$$

where T refers to the dosage time and ψ_s is often referred to as the dosage or exposure, and the subscript s is introduced as a reminder that all sources and puffs are included in the calculation. The average concentration over the time interval T is then found by dividing ψ_s by T. The dosage integral in equation [11] is approximated in CITPUFF by the use of a sampling function. The method of calculation described above will also simulate the concentration field from a continuous source, provided the series of discrete puffs overlap along the variable plume axis with sufficient density. The last section considers simulation of the continuous plume in more detail, and also compares the predictions of CITPUFF to those of other models.

CITPUFF MODEL—SPECIFIC MODEL COMPONENTS

Grid System and Basic Computational Unit

The CITPUFF model uses a Cartesian coordinate system for both input and output. The maximum allowable size of the computational grid in the current version of CITPUFF (as implemented on the CSU Cyber 720 computer) is approximately 6400 grid points (e.g., an 80 by 80 grid area).

The wind field required to drive the CITPUFF model must be specified in the form of horizontal (u and v) wind vector components at each Cartesian grid point of the computational grid. The wind field can be updated after each basic computational unit (1-hr intervals in the current version of CITPUFF). The source of the wind fields used in CITPUFF and the subsequent interpolation scheme used for advecting puffs are outlined in the next section.

The basic computational unit in the current version of CITPUFF is 1 hr. The model is organized so that the minimum time average that can be obtained directly is a 1-hr average. Emission characteristics and meteorology can be updated every hour, with the input values taken as representative of 1-hr averages for the given period of time.

Factors such as puff release rate, sampling frequency, time and length of basic advection steps, are designed to support the 1-hr basic computational unit. The CITPUFF model is flexible, and if required can be adjusted for alternative basic computational units.

Meteorology

The CITPUFF model requires the following meteorological inputs:

a. Stability class and mixing depth specified at hourly intervals
b. Horizontal (u,v) wind components (at a standard height above ground level) specified at each of the wind field grid points at hourly intervals
c. Ambient temperature (in °K) to calculate plume rise for any sources in the analysis area at hourly intervals.

In the current version of CITPUFF a single stability class mixing depth and ambient temperature are specified for the analysis area being considered. The gridded wind components (u and v) currently used to drive CITPUFF are produced by the complex-terrain wind field model WINDS (Fosberg et al. 1976). It is also possible to use the u and v components from a three-dimensional wind model, which like WINDS is a component of the Topographic Air Resources Analysis System (TAPAS) (Fox et al. 1984). The WINDS model is a grid-based, two-dimensional diagnostic model. The model relies on simplified solutions to complex equations that characterize the major controlling physical processes that influence wind flow over complex terrain. The model does not attempt to solve time-dependent, predictive, atmospheric fluid and thermodynamic equations that require large initial data fields and extensive computer resources. Instead, the model simulates the two-dimensional, horizontal wind flow over complex terrain by combining the terrain-induced flow concept described by Anderson (1971) and the thermally induced wind flow processes described by Fosberg et al. (1972). The WINDS model handles subsynoptic situations where a characteristic prevailing wind can be used to initialize the entire grid. Intermittent, decoupled, or separated flow simulations are not within the scope of the model. Hence, there are limitations on the severity of topographic variation that can be addressed by the model. The model was designed, and is best applied, to accommodate grid point spacing of one-half to several kilometers.

The primary model inputs are:

- Elevation at each grid point
- Vegetation/land cover class at each grid point
- Temperatures and associated heights of two layers of the atmosphere that define the atmospheric temperature profile
- Influencing wind direction and wind speed (and any available wind observations).

The WINDS model calculates a resultant wind field in two phases. Phase 1 accounts for the effect of major terrain features on the influencing wind throughout the depth of the boundary layer. Phase 2 modifies the wind field calculated in Phase 1 by accounting for wind perturbations caused by the actual terrain, thermal, and frictional forces within a shallow, near-surface air layer. In both phases, mass is conserved within defined horizontal and vertical dimensions and nonlinear forces are not calculated.

The primary output of the model used in CITPUFF is a digital file that contains both the u and v wind components at each grid point of the computation grid for a selected analysis area. The WINDS model as well as other TAPAS models outputs are formatted in TAPAS-structured files (Childs and Marlatt 1981). CITPUFF is designed to directly read and interpret TAPAS-structured files.

Trajectory Calculation

The trajectory calculation requires two gridded wind field data sets that represent conditions occurring 1 hr apart. These wind component data sets are used to construct trajectories at a particular place on the grid at a particular time, by performing a bilinear interpolation in space, followed by a linear interpolation in time.

The trajectory for the u component is illustrated following the original presentation in Hales et al. (1977). Let the times of two consecutive wind fields be t and $t+\Delta t_w$, respectively. The interval between wind maps, Δt_w, is 1 hr in the current version of CITPUFF. Referring to figure 1, it is necessary to calculate $u(t+\Delta t,p,q)$, given $u(t,0,0)$, $u(t,1,1)$, $u(t+\Delta t_w,1,1)$, $u(t+\Delta t_w,0,0)$, etc., where Δt is the advection time interval (time step) and p and q represent grid points. In this case,

$$\begin{aligned} u(t+\Delta t,p,q) = {} & \left(1-\frac{\Delta t}{\Delta t_w}\right)[(1-p)(1-q)u(t,0,0) \\ & +(1-p)qu(t,0,1)+p(1-q)u(t,1,0)+pqu(t,1,1)] \\ & +\frac{\Delta t}{\Delta t_w}[(1-p)(1-q)u(t+\Delta t_w,0,0)+(1-p)qu(t+\Delta t_w,0,1) \\ & +p(1-q)u(t+\Delta t_w,1,0)+pqu(t+\Delta t_w,1,1)] \end{aligned}$$

The same procedure is used for determining $v(t+\Delta t,p,q)$.

Winds computed in this manner from grid values are used in a two-step iteration method to calculate trajectory steps. The manner in which the trajectory step is calculated from time t to time $t+\Delta t$ for a particle located at $[x(t),y(t)]$ in figure 1 is such that a particle so transported would arrive at (x_1,y_1) at time $t+\Delta t$ if the wind remained constant. However, because the wind would change along the trajectory, the actual location $[x(t+\Delta t),y(t+\Delta t)]$ of the particle would be at some nearby point. To better approximate this location, the wind at (x_1,y_1) at time $t+\Delta t$ is also calculated and used to calculate a second advection step to (x_2,y_2). The $[x(t+\Delta t),y(t+\Delta t)]$ is assumed to lie halfway between $[x(t),y(t)]$ and (x_2,y_2). The equations for calculating $x(t+\Delta t)$ are as follows:

$$x_1 = x(t) + u(t,x(t),y(t))\Delta t$$

$$x_2 = x_1 + u(t+\Delta t,x_1,y_1)\Delta t$$

$$x(t+\Delta t) = 0.5[x(t)+x_2]$$

In exactly the same way, $y(t+\Delta t)$ is calculated using the v component of the wind.

Puff Dispersion

The CITPUFF model contains three user options for calculating puff dispersion: Pasquill stability (Hales et

al. 1977), Power Plant Siting Program (PPSP) dispersion coefficients (Brower 1982), and 22.5° sector dispersion (EPA 1981).

Pasquill-Gifford Stability Based Dispersion

The Pasquill-Gifford-Turner stability based dispersion approach is the primary method used in most CITPUFF applications (Hanna et al. 1982). The diffusion of the puffs relative to their trajectory is described by distance-dependent values of σ_y and σ_x for distances of up to approximately 100 km. The growth of a puff along the puff trajectory distance s from the source is represented by:

$$\sigma_y(s+\Delta s)=\sigma_y(s)+\Delta s\frac{d\sigma_y}{ds}\bigg|_{s=\Delta s/2}$$

$$\sigma_z(s+\Delta s)=\sigma_z(s)+\Delta s\frac{d\sigma_z}{ds}\bigg|_{s=\Delta s/2}$$

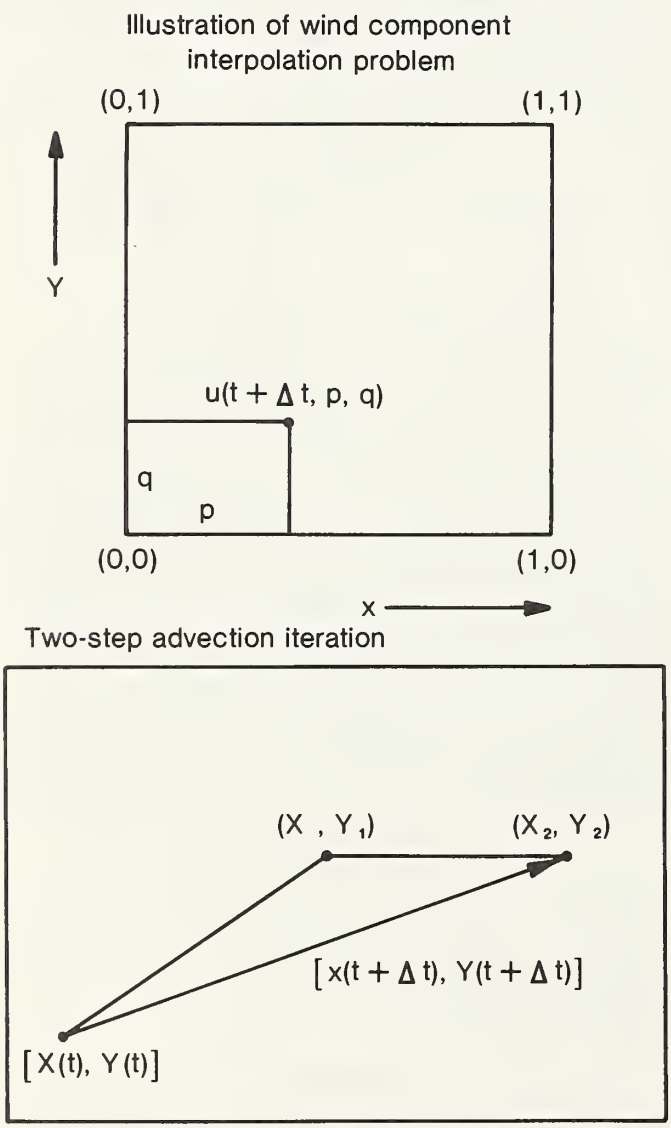

Figure 1.—Interpolation of wind components and analysis of the two-step advection iteration.

Similar equations for σ_y and σ_z as a function of travel time are also available to calculate dispersion as a puff travels beyond approximately 100 km from the source.

The distance functions used in CITPUFF for Pasquill-Gifford-Turner atmospheric stability classes A (very unstable) through F (very stable) have the following form:

$$\sigma_y = as^b \quad , \quad \sigma_z = cs^d$$

where the coefficients a, b, c, and d correspond to a given Pasquill stability category, as shown in table 1. These coefficients were obtained by approximating the σ_y and σ_z dispersion curves of Turner (1970). Values of s and the corresponding values of σ_y and σ_z are in meters. In CITPUFF, these dispersion functions are implemented as derivatives along the puff trajectory path.

For travel distances greater than 100 km, time-based formulations are more appropriate than distance-based formulations (Hanna et al. 1982). The CITPUFF model contains a time formulation given by Heffter (1965):

$$\sigma_y = 0.5t \quad , \quad \sigma_z = \sqrt{2K_z t}$$

where t is in seconds, σ_y and σ_z are in meters, and K_z is the vertical eddy diffusivity. Following Heffter, K_z has been set at 5 m²/s in the CITPUFF model. Selection of the time-related dispersion parameter is a user option in CITPUFF. The user assigns a time, depending on the wind speeds in the analysis area, that corresponds to the transport of pollutants approximately 100 km from the source.

Power Plant Siting Program Dispersion

An option exists in CITPUFF to select the dispersion coefficients σ_y and σ_z used in the Maryland Power Plant Siting Program (PPSP) (Brower 1982), as adapted from Gifford (1975). These coefficients, initially suggested by Briggs, following, in part, Smith (1968), are based on empirical formulations derived from available diffusion data from buoyant sources with ground and elevated releases. Briggs does not recommend their use beyond a few kilometers from the source. Table 2 presents the downwind distance-dependent dispersion coefficients as a function of stability as defined by Briggs. Briggs' A coefficients are appropriate for most unstable atmospheric conditions, while Briggs' F coefficients are appropriate for most stable conditions. To select the appropriate PPSP dispersion parameter, it is necessary to evaluate which Briggs stability category is most appropriate for desired modeling conditions. This must be done external to the CITPUFF model using the method described in Brower (1982). Appendix A includes a comparison between PPSP and the Pasquill-Gifford-Turner dispersion approaches.

The PPSP dispersion parameters, as applied in CITPUTT, have the forms given in table 2. Again they are implemented in differential forms. The user has the option of specifying a time at which the time-dependent dispersion coefficients are applied.

Table 1.—Coefficients for Pasquill stability based dispersion parameter formulas (from Hales et al. 1977).

Pasquill stability category	σ_y a	σ_y b	σ_z c	σ_z d
A (1)	0.36	0.9	0.00023	2.10
B (2)	0.25	0.9	0.058	1.09
C (3)	0.19	0.9	0.11	0.91
D (4)	0.13	0.9	0.57	0.58
E (5)	0.096	0.9	0.85	0.47
F (6)	0.063	0.9	0.77	0.42

Table 2.—Horizontal (σ_y and vertical (σ_z) dispersion coefficients recommended by Briggs (Gifford 1975) as a function of downwind distance, x (in meters).

Sigma curve identifer	σ_y	σ_z
1. BRIGGS A	$0.22x(1+0.0001x)^{-1/2}$	$0.20x$
2. BRIGGS B	$0.16x(1+0.0001x)^{-1/2}$	$0.12x$
3. BRIGGS C	$0.11x(1+0.0001x)^{-1/2}$	$0.08x(1+0.0002x)^{-1/2}$
4. BRIGGS D	$0.08x(1+0.0001x)^{-1/2}$	$0.06x(1+0.0015x)^{-1/2}$
5. BRIGGS E	$0.06x(1+0.0001x)^{-1/2}$	$0.03x(1+0.0003x)^{-1}$
6. BRIGGS F	$0.04x(1+0.0001x)^{-1/2}$	$0.016x(1+0.003x)^{-1}$

22.5° Sector Dispersion

An option also exists in CITPUFF to choose the 22.5° sector dispersion algorithm, as applied in the EPA COMPLEX I model (EPA 1981). The puff is dispersed horizontally within a 22.5° arc in the direction of the local wind, dependent on distance from the source. Vertical dispersion is calculated identically to the distance-related σ_z of the COMPLEX I model. Because the COMPLEX I approach is applied for calculating σ_z, the user is cautioned that the initial value of σ_z is assumed to be 1 m. The user cannot input initial σ_z values greater than 1 m when the 22.5° sector option is applied.

The method used to assign ground-level concentration values to grid receptors from the calculated sigma values is the same as that used in all other CITPUFF options. In addition, the user has the option of specifying a time at which the time-dependent dispersion coefficients are applied.

Definition of Initial Sigma Values

CITPUFF allows for the specification of initial sigma values, σ_{yo} and σ_{zo}, at the pollutant source ($s=0$). Area/volume source distributions can be specified by appropriate choices of the initial sigma values. With some approximation, this allows the simulation of various types of complex sources including forest fires and surface mines.

Effective Emission Height

To complete the solution for ground-level concentration for a discrete puff (equation [10]), an effective pollutant source height (h) must be calculated from the physical parameters associated with the source emission. The CITPUFF model has incorporated plume rise formulations from the EPA Multiple Point Gaussian Dispersion Algorithm with Optional Terrain Adjustment (MPTER) (EPA 1980) to calculate the effective emission height from each source. The implemented plume rise algorithm is an adaptation of Briggs' formulations and accounts for varying stability, momentum and buoyancy rise, and stack downwash. The physical source parameters required as input to plume rise calculations include emission type, source location, emission rate, physical stack height, stack gas temperature, stack diameter, stack gas exit velocity, and ambient temperature and wind. A thorough description of the plume rise equations is available in EPA 1980.

If appropriate stack or source parameters are unknown, a user-estimated effective plume height can be entered directly into the CITPUFF model.

Terrain Height Adjustment

Following the approach used by other models applied in complex terrain (Egan 1975, Schulman and Scire 1980, Lavery et al. 1983), stability-dependent plume path coefficients are used to calculate the effects of terrain elevation on the height of the plume centerline.

The terrain-corrected effective stack height, h_t, above the terrain is calculated from

$$h_t = h - (1-\tau)(\text{minimum}\{h, E_R - E_P\})$$

where

$h = h_s + \Delta h$ is effective stack height above stack base elevation,
h_s = physical stack height,
Δh = plume rise,
E_R = receptor elevation,
E_p = stack base elevation,

τ = the plume path coefficient, whose value is given in the following tabulation for different stability classes:

Stability class	Plume path coefficient, τ
A	0.5
B	0.5
C	0.5
D	0.5
E	0.3
F	0.3

For neutral and unstable conditions the plume is lifted one-half of the difference between the elevation of the receptor and the elevation of the stack base, with the additional restriction that the plume always be at least half the height above the ground that it would be with no topography. Under stable conditions the one-half condition is replaced by a one-third condition.

The appropriateness of plume path corrections to all situations is uncertain and, therefore, the user has the option of inputting any desired set of values if the default values are considered inappropriate. Obviously, selection of $\tau = 1$ will yield a flat, non-terrain-lifted plume.

Wind Power Law Adjustment

CITPUFF uses a power law function of the form:

$$\frac{u(z)}{u_R} = \left(\frac{z}{z_R}\right)^p$$

to adjust the winds input from the WINDS model (at $z = z_R$) to the height required by the plume rise calculation for puff trajectory calculations. The default power law exponents within CITPUFF for each stability category are:

Stability class	Power law exponent
A	0.15
B	0.15
C	0.20
D	0.25
E	0.40
F	0.60

The user has the option to change the power law exponent if desired.

Effect of Mixing Depth and Puff Fumigation

Mixing depth (H) is taken into account by using the technique of multiple reflections of the puff when significant pollution reaches the specified level as first established by Bierly and Hewson (1962). If the mixing depth height is taken as H, this technique leads to the following equation for the puff concentration at ground level:

$$\bar{\chi}(x,y,0) = \frac{2Q}{(2\pi)^{3/2}\sigma_y^2\sigma_z} \exp\left(\frac{-r^2}{2\sigma_y^2}\right) \exp\left(\frac{-kx}{\bar{u}}\right) \left\{\exp\left[-\frac{1}{2}\left(\frac{h}{\sigma_z}\right)^2\right] \exp\left[-\frac{1}{2}\left(\frac{2H-h}{\sigma_z}\right)^2\right]\right\} \qquad [12]$$

For the case of uniform vertical distribution within H this becomes:

$$\bar{\chi}(x,y,0) = \frac{Q}{2\pi H\sigma_y^2} \exp\left(\frac{-r^2}{2\sigma_y^2}\right) \exp\left(\frac{-kx}{\bar{u}}\right) \qquad [13]$$

In the current version of CITPUFF, the user specifies one of two possible algorithms based on equations [12] or [13].

Puffs with an effective emission height above the user-defined mixing height will not contribute to ground-level concentrations. If, however, the mixing height at some later time period becomes greater than the height of these puffs, they then begin to contribute to ground-level concentrations, although their effective release height remains unaltered. For simplicity, CITPUFF assumes that puffs residing below the mixing depth can diffuse through the maximum depth H encountered by the puffs at any given time of simulation.

Puff Sampling Function

The dosage integral in equation [11] for a single source is approximated in CITPUFF by a summation of the form

$$\psi_s = \int_{t_o}^{t_o+T} \bar{\chi}dt = \frac{1}{\bar{u}}\int_{x_o}^{x_o+x} \bar{\chi}dx \cong \sum_{j=1}^{N}\left(\frac{\bar{\chi}\cdot\delta x}{\bar{u}}\right)_j \qquad [14]$$

where the approximations $x = \bar{u}t$ and $dx = \bar{u}dt$ are used. The summation process is similar to approximate integration by the trapezoidal rule, except that concentration at the end of a time interval j, $\bar{\chi}_j$ is assumed to prevail over the entire time interval $(\delta t_j = \delta x_j/\bar{u}_j)$. The summation in equation [14] is obtained by periodic sampling of the puffs. Depending upon the number of intervals or sampling frequency used, the approximation may converge to the integral at any desired level of accuracy.

The sampling frequency algorithm developed by Start and Wendell (1974) is used to evaluate the distance increment form used in equation [14]. During periods of strong winds, this algorithm allows the puffs to be sampled several times during an advection step. At low speeds, puffs will be sampled less frequently.

To determine the contribution of each puff to ground-level pollutant concentration, the radius of each puff is determined by the relation:

$$R_p = 2\sigma_y\left\{-2\ell n\left(\frac{\bar{\chi}_{min}}{\bar{\chi}_p}\right)\right\}$$

where

$\bar{\chi}_{min}$ = the minimum concentration of interest, and

$\bar{\chi}_p$ = the concentration at the puff center.

The ground-level concentration is computed for each time step and accumulated over the entire time of the simulation for each grid point that lies within the radius of influence of each puff. If $\bar{\chi}_p \leqq \bar{\chi}_{min}$ (as defined by the

user), the puff is considered to have become so diluted that it no longer can be considered as contributing to the ground-level concentration. Under these conditions the puff is eliminated from further calculations to conserve computer requirements. A puff that is transported beyond the analysis area grid is also eliminated from further calculations. A maximum of 500 puffs can be considered simultaneously in CITPUFF.

EXAMPLE APPLICATION OF CITPUFF

Overview

An analysis area in northwestern Colorado was chosen to provide an example application of CITPUFF. Emission from two hypothetical oil shale sources within the analysis area (the Piceance Basin) were studied.

Figure 2, a map of the analysis area, includes the location of the two sources and nearby landmarks. A summary of the primary spatial, temporal, and meteorological boundary conditions applied in this example application of TAPAS (WINDS and CITPUFF models) includes:

- Grid dimensions: x = 81; y = 61
- Grid spacing: 2-min grid intervals
- Approximate distance between grid points: x = 2.86 km; y = 3.70 km
- Terrain and land cover at each grid point (terrain extracted from data tapes using the TAPAS Terrain Access Routines (NOAA/EDIS/NSGDC 1980); land cover was manually digitized)
- Surface temperature at 1800 m: 20° C (293° K)
- Influencing wind: west-southwest at 4 m/s (10 m above surface)
- Sampling period: 12-hr steady-state wind condition
- Assumed mixing depth: 4300 m above mean sea level
- Assumed stability for Pasquill stability related dispersion: Class E (stable) (Pasquill-Gifford dispersion coefficients assumed)
- Puff release frequency: 10 min
- No deposition or decay of pollutants was considered in the CITPUFF model run
- Number of minutes between puff sampling: Determined within model
- Ground-level concentrations were output only at the end of the 12-hr period (PTIME(1) = 12)
- Default values for terrain adjustment factors and wind power law were assumed
- Puff dispersion was switched from distance- to time-related calculations at 3-hr
- A 12-hr simulation with no variation in meteorological conditions throughout the period was performed

An elevation contour map of the analysis area is provided as figure 3. A velocity vector plot of the WINDS

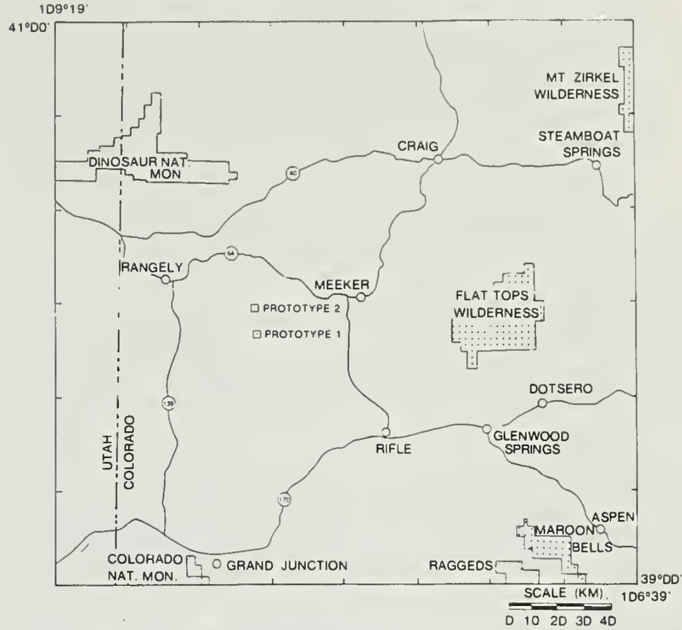

Figure 2.—Base map of the analysis area considered in the example CITPUFF analysis.

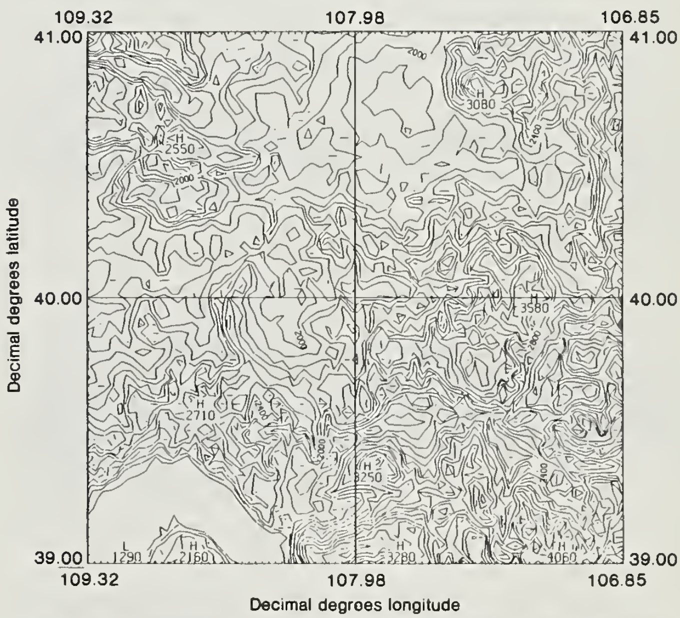

Figure 3.—Elevation contour map of analysis area (contour interval—100 m).

model results for a west-southwest influencing wind condition are provided in figure 4.

Elevated sulfur dioxide (SO_2) emission data from the two oil shale sources considered in this example are listed below. To account for the horizonal and vertical distribution of emissions from individual plant processes, elevated emissions from these oil shale sources were assigned initial σ_y and σ_z of 125 m and 75 m, respectively. Since no engineering information was available on stack parameters, CITPUFF was not asked to calculate plume rise in this example. All elevated emissions were assumed to be emitted at a 300-m effective plume height.

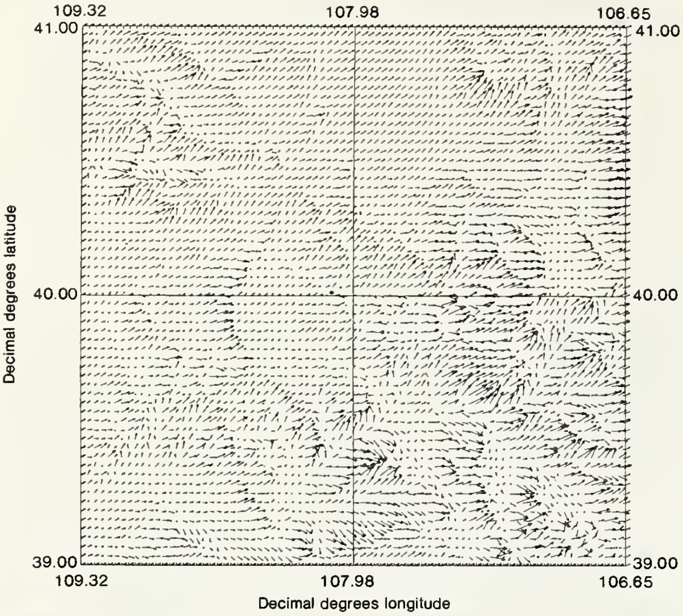

Figure 4.—Velocity vector plot of west-southwest wind field for the example analysis area (based on influencing wind of WSW at 4 m/s).

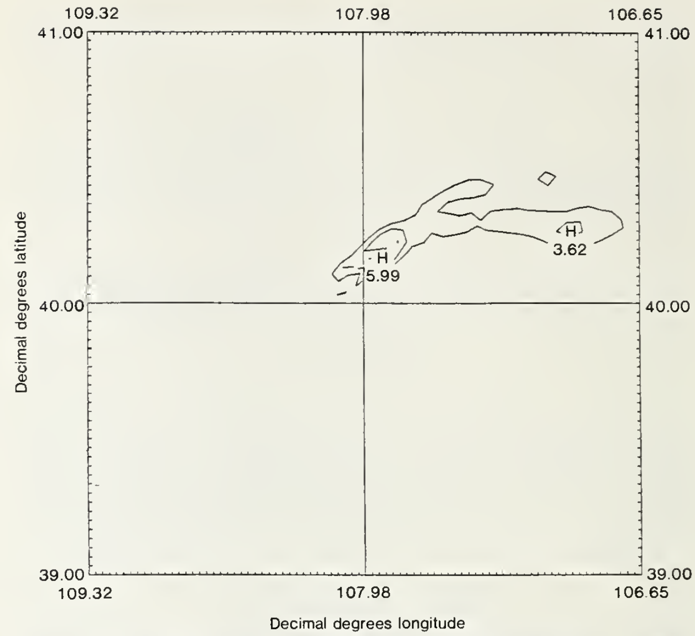

Figure 6.—SO_2 ground-level pollutant concentrations ($\mu g/m^3$) resulting from this example CITPUFF analysis.

Source 1: Prototype 1 — 101 g SO_2/s (Cb-MIS process)
Source 2: Prototype 2 — 67 g SO_2/s (Union-B DM/SR process)

A puff trajectory plot of the analysis results is provided as figure 5. A contour plot of ground-level SO_2 pollutant concentrations for the example 12-hr period is provided as figure 6.

CONSIDERATIONS OF MODEL VALIDITY

The CITPUFF model is designed to add two features of dispersion in complex topography that are not incorporated in other available Gaussian-based models. These are, first, the accommodation of a space- and time-varying wind field and, second, the availability of added correction factors to adjust the plume path beyond the capacity of the flow field. Both of these features are needed to simulate conditions in complex terrain. A choice of three diffusion parameterizations is also provided. Adjustments to diffusion coefficients can be easily accomplished if a consensus is established on the most appropriate coefficients. However, this model can not be expected to resolve all controversies associated with modeling dispersion in complex topography. This section describes the capabilities and limitations of the CITPUFF model. It does not provide assurance that the model will always be correct or that it has been totally validated. However, to the extent that the model incorporates conventional procedures (Gaussian form, Pasquill-Gifford diffusion and its variants), one can estimate its likely validity.

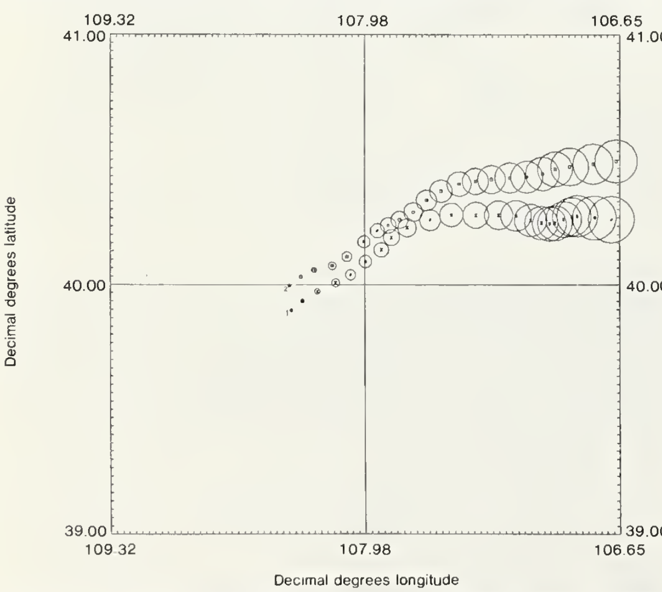

Figure 5.—Puff trajectory plot of the two sources modeled in this example CITPUFF analysis.

Uncertainty about model performance should be a keynote in most model applications and will remain so in air quality applications for the foreseeable future (Fox 1984). For the particular case of models that treat dispersion for long distances in complex terrain, there is no adequate data base upon which to evaluate performance. However, this section will summarize the status of knowledge, identify where CITPUFF resides within that status, and suggest some limitations on its use and the utility of model output.

Dispersion Accuracy

The Pasquill-Gifford-Turner dispersion formulation, upon which CITPUFF dispersion is based, has been repeatedly defined as state of the art (Pasquill 1974, EPA 1978, Bass et al. 1979). However, recent advances in the understanding of boundary layer physics (Nieuwstadt and Van Dop 1982) suggest that under convective (unstable) conditions, the formulation is fun-

damentally incorrect, and under stable conditions the physics of the boundary layer may be so complex that simple models are inadequate. Recently, Weil and Brower (1982) have incorporated some of these modern concepts into a model. Model results show significantly improved performance. A major limitation of the Weil and Brower (1982) approach, however, is the need for significantly increased meteorological data to drive the model. The current EPA complex-terrain model development program (Lavery et al. 1982, 1983; Strimaitis et al. 1983) is systematically evaluating the effects of topography on ground-level concentration of plumes. Results from this study suggest that improvement in the accuracy of ground-level predictions can result from the addition of plume path correction factors and determination of dispersion coefficients based on local measurements of the turbulence. Because local measurements are generally not available, it is necessary to rely on conventional dispersion schemes. After considering comparisons of existing techniques, this study concludes that COMPLEX I does a better job of simulating the field data than any of the other routinely available models (Lavery et al. 1982). COMPLEX I is distinguished by the fact that it allows the plume to disperse horizontally through an arc of 22.5° under all stabilities. That such a simple approximation works is likely due to the presence of rather large-scale meanders in the flow in complex terrain under all stabilities.

The CITPUFF model provides the user with a choice of three available dispersion schemes: Pasquill-Gifford, PPSP, and 22.5° sector. Since all of the schemes have had extensive evaluation, it is not necessary to reestablish their validity. Of concern, however, is how well the discrete puff algorithm in CITPUFF is able to simulate the Gaussian plume and, therefore, how well the dispersion algorithm is implemented. For example, an important requirement of CITPUFF is that it provide an adequate approximation of the continuous point source solution in situations where use of the continuous point source solution is justified.

Adequate representation by a puff model of the continuous point source solution, particularly within 10 km of the source, depends on the puff release and puff sampling rates used. Guidance in selecting values of these parameters has been provided by an investigation using the MESODIF model conducted by Start and Wendell (1974). This investigation showed that if the puff travel distance between samples is restricted to less than 2.4 km, and the puff release interval is no more than 10 min, the puff model will provide an adequate approximation of the continuous point source solution for all but isolated cases characterized by very strong hourly averaged wind speeds. A release rate of six puffs per hour was found to provide a reasonable compromise between the increased accuracy in representing the continuous point source solution that could be achieved by more frequent puff releases, and the increased computational time and costs involved in increasing the puff release rate. For long-term model applications (on the order of a year) a rate of three puffs per hour was shown to provide a reasonable approximation.

CITPUFF (using the Pasquill-Gifford dispersion option) and the continuous point source equation were compared to find the normalized ground-level concentrations predicted by each approach over flat terrain under various stability conditions. In all cases, CITPUFF was applied assuming

puff release rate = 6 puffs per hour
basic advection step = 10 min
puff sampling time = 2 min.

A wind speed of 2.78 m/s was tested under Pasquill stability classes B, C, D, E, and F. An additional wind speed of 11.11 m/s was also tested under the D stability condition. Comparisons were made up to 25 km from the source.

Figures 7 through 11 present the results of the CITPUFF versus continuous point source Gaussian solutions for Pasquill stability conditions B, C, D, E, and F, respectively. The comparisons indicate that CITPUFF provides a very close approximation of the continuous point source solution under the tested conditions.

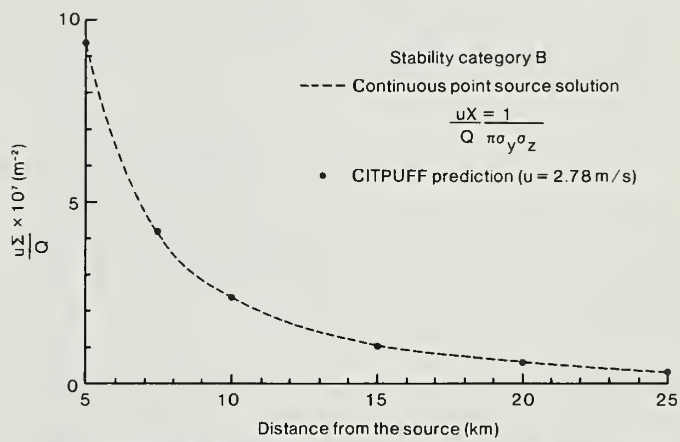

Figure 7.—Comparison of continuous point source solution and CITPUFF (Pasquill dispersion parameters) solution over flat terrain; stability B—unstable.

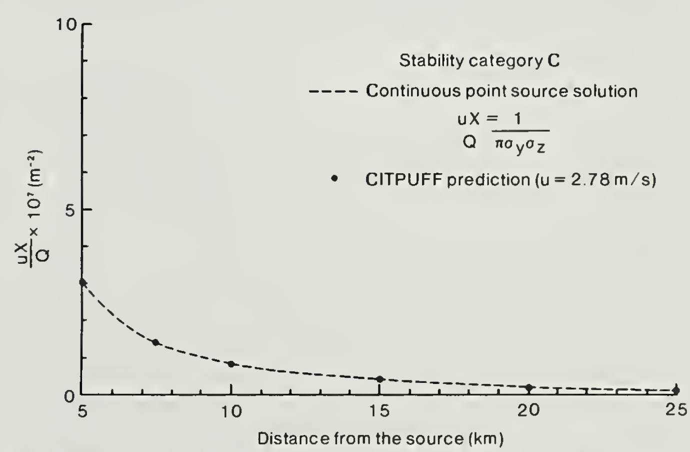

Figure 8.—Comparison of continuous point source solution and CITPUFF (Pasquill dispersion parameters) solution over flat terrain; stability C—slightly unstable.

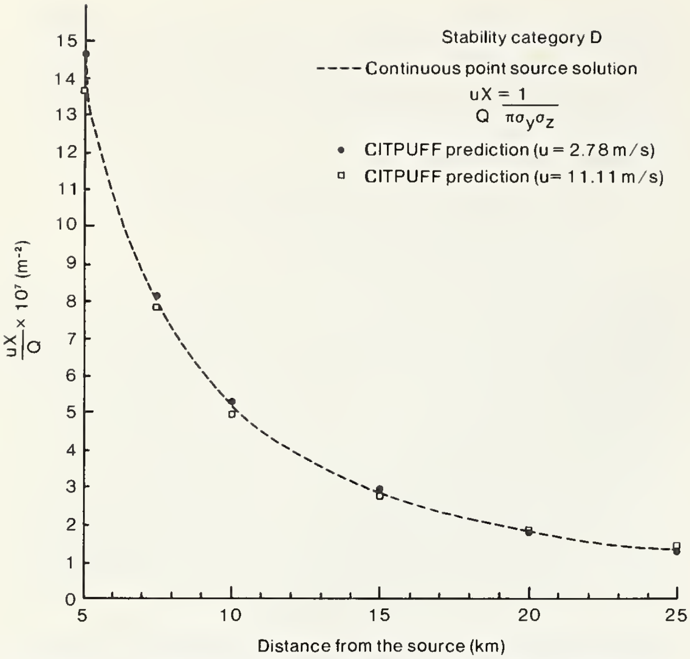

Figure 9.—Comparison of continuous point source solution and CITPUFF (Pasquill dispersion parameters) solution over flat terrain; stability D—neutral

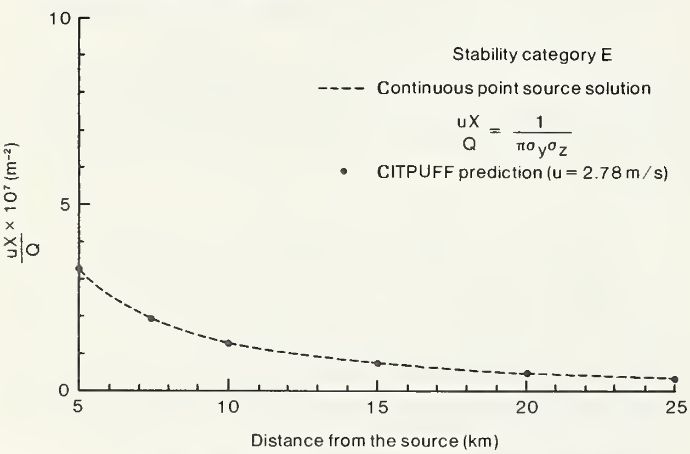

Figure 10.—Comparison of continuous point source solution and CITPUFF (Pasquill dispersion parameters) solution over flat terrain; stability E—slightly stable.

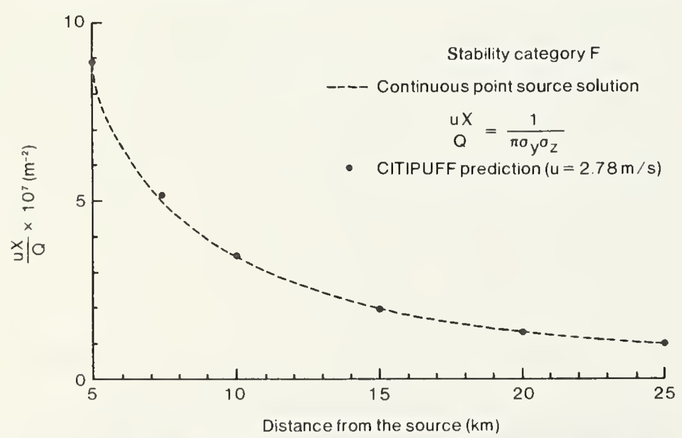

Figure 11.—Comparison of continuous point source solution and CITPUFF (Pasquill dispersion parameters) solution over flat terrain; stability F—stable.

Plume Path Correction Factors

A primary focus of current research is on how a plume behaves as it encounters simple topographic elements. This research indicates that the first requirement for predicting reasonable ground-level concentrations is simulation of the correct plume trajectory (Lavery et al. 1982). The puff trajectories calculated by the CITPUFF model depend on the wind field provided by the WINDS model (or any other method used to generate a grid-based wind field). For applications with WINDS the plume trajectory is limited by the two-dimensional nature of the WINDS model. WINDS predicts flows parallel to the topography at the ground surface and hence contains no vertical velocity independent of the orographic lifting. Thus, the flow field is unable to resolve any vertical adjustment that the puff may actually undergo as it approaches terrain. In an extensive analysis of this problem Bass et al. (1981) concluded that making stability-dependent plume height adjustments in response to the presence of terrain, is appropriate.

Correct vertical adjustment of the puff, however, may require additional considerations. EPA studies indicate that the local Froude number ($F = U/Nh$ where $N = [(g/\theta)\cdot(d\theta/dz)]^{1/2}$) associated with the height of the local terrain element, determines whether the plume goes toward, around, or over the terrain. In fact, models have recently been developed to make precise numerical evaluations of ground-level concentration under each of these regimes. However, the needed meteorological information is not available in the applications of interest to the targeted users of TAPAS. Furthermore, the concept of precise plume behavior has not been generalized to anything more complex than a single isolated hill considering wind speed (not direction) and temperature variations. Continuing research will likely yield greater understanding and better data. Options provided in CITPUFF provide the model user with the ability to use or not use plume path correction factors. As more precise plume adjustment factors are developed, they can be incorporated into CITPUFF.

Because the CITPUFF model operates with a modeled wind field, it is appropriate to discuss the implications of plume path correction factors within this wind field. The absence of vertical velocity in the model leads to a tendency for winds to flow around topography. The path correction features cause the puff centerline to decend toward the topography. Thus, their use is a conservative factor that tends to cause higher values of ground-level concentration than would otherwise be calculated.

Comparison of CITPUFF to EPA COMPLEX I and COMPLEX II

Overview

Currently (1984) EPA does not recommend any model for application in complex terrain (EPA 1978). Furthermore, they suggest that appropriate cautions should be applied when using Gaussian plume models beyond 50 km. However, in order for the federal land manager to

meet the requirement that air quality related values of Class I areas be protected (Fox et al. 1982), model results must be used.

Although no model is recommended, the EPA does suggest that COMPLEX I and COMPLEX II can be used as screening models. In particular, recent results from the small hill study (Strimaitis et al. 1983) indicate that COMPLEX I comes closer to predicting maximum ground-level impacts than does COMPLEX II. COMPLEX II appears to be overly conservative. A comparison of CITPUFF against COMPLEX I and COMPLEX II for an idealized situation is provided below.

COMPLEX I and COMPLEX II

COMPLEX I and COMPLEX II are multiple point-source diffusion models developed by the EPA for application in rural and complex terrain (Irwin and Turner 1983). Both models have been used for regulatory purposes. The models are best applied within 50 km of the source. Beyond 10 km, mesoscale influences, primarily spatial wind variation, may affect model results, particularly in complex terrain. For a user-defined time period, the COMPLEX models assume that a single, fixed, wind direction and speed (defined at the source) transports and disperses the model plumes. A series of options and variables are available within the models to account for plume terrain interactions, stability-related wind profile, plume rise, emission rate, receptor locations, and other parameters. The basic difference between COMPLEX I and COMPLEX II is the treatment of horizontal dispersion (σ_y) COMPLEX I assumes that pollutants are uniformly distributed over a 22.5° sector. COMPLEX II assumes horizontal dispersion based on Pasquill-Gifford estimates (Turner 1970). For example, based on these dispersion considerations, COMPLEX I will provide lower downwind centerline ground-level concentrations than COMPLEX II under stable conditions.

Model Comparisons on Theoretical Flat and Mounded Terrain

COMPLEX I, COMPLEX II, and CITPUFF were all applied to simulate ground-level concentrations for theoretical flat and mounded terrain fields. A single-source emission of 100 g/s with an effective stack height of 300 m (final plume rise) was assumed. An influencing wind of 4 m/s from the west (measured 10 m above the surface) was chosen. A stable condition (Class E stability) was assumed for the comparison.

Both flat and mounded simulated terrain data were compiled for the test. The mounded terrain field consisted of two Gaussian-shaped hills, one centered at 30 km from the source and the other centered at 69 km. A cross-section schematic of the mounded terrain is provided in figure 12. For CITPUFF modeling, the terrain was defined within a two-dimensional grid of $x=75$, $y=21$, with a distance between grid points of 1.5 km. Receptors for COMPLEX I and COMPLEX II were located every 3 km downwind to 99 km from the source.

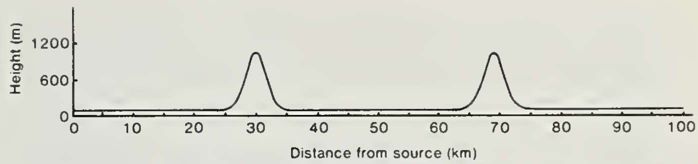

Figure 12.—Cross section of mounded terrain data for EPA COMPLEX/CITPUFF comparisons.

COMPLEX I and COMPLEX II were applied as recommended for regulatory purposes. The suggested configuration of COMPLEX I and II (to conform to the EPA complex terrain concepts determined at the Chicago Workshop on Air Quality Models in 1980, EPA 1981) includes the following:

1. terrain adjustment factors (0.5, 0.5, 0.5, 0.5, 0.0, 0.0, for A through F stabilities),
2. buoyancy-induced dispersion,
3. plume heights no closer than z_{min} (10 m) to receptors,
4. wind power-law coefficients used in lieu of other justifiable site-specific data (0.1, 0.15, 0.2, 0.25, 0.3, 0.3, for A through F stabilities).

Three configurations of CITPUFF as defined by variations in the dispersion coefficients (Pasquill-Gifford, PPSP, and 22.5°) were compared. Point-source emissions are modeled using initial σ_y and σ_z values of 1.0 m and 1.0 m, respectively.

Results of flat terrain comparisons.—The results of CITPUFF-COMPLEX centerline comparisons for flat terrain are plotted in figure 13. CITPUFF (22.5° sector) yields the lowest ground-level estimates of all modeling at all receptors. COMPLEX I yields the next lowest estimates of ground-level concentrations. COMPLEX II yields ground-level concentration results that are generally higher by a factor of five than COMPLEX I estimates. CITPUFF (Pasquill-Gifford) estimates generally fall between COMPLEX I and COMPLEX II values. CITPUFF (PPSP) estimates are high near the source, but beyond 66 km CITPUFF (PPSP) estimates fall below COMPLEX II estimates. Beyond 50 km from the source, all results presented fall within a factor of five range.

Results of mounded-terrain comparisons.—Model results for mounded-terrain runs are plotted in figure 14. Basic differences exist in the way COMPLEX I and II and CITPUFF account for terrain under stable conditions. COMPLEX I and II, as applied, assume terrain adjustment coefficients of 0.0 under E stability. Based on this assumption, ground-level concentrations for terrain well above the plume centerline are not calculated. The highest ground-level concentrations are calculated where the plume impacts the terrain. Note that no values are plotted for the COMPLEX models at the highest terrain receptor in figure 14, because the model does not calculate a value at this point. To continue plume transport beyond high terrain, the COMPLEX models assume that no terrain exists, and they continue transport and dispersion of the plume effectively through the mountain and beyond assuming the initially defined wind speed and direction.

The CITPUFF model depends on terrain-related wind fields (such as provided by the WINDS model) to provide an estimate of transport winds. Variations in the transport wind vector occur as terrain is encountered. In addition, a terrain adjustment factor of 0.3 is commonly used for E stability in the Pasquill-Gifford-Turner and PPSP versions of CITPUFF. This factor indicates that the plume is lifted approximately one-third of the difference between the elevation of the receptor and the elevation of the stack base, with the additional restriction that the plume always be at least half the height above the ground that it would be with no topography. Ground-level concentrations are therefore provided for all grid points in the plume's influence. The terrain adjustment and wind power law adjustment factors that are normally used in the 22.5° sector version of CITPUFF are the same as applied in COMPLEX I.

The CITPUFF (22.5° sector) model yields the lowest ground-level concentration in the mounded terrain test. COMPLEX I yields the next lowest values. COMPLEX II yields results a factor of five or higher than COMPLEX I. CITPUFF (Pasquill-Gifford) results are similar to, yet slightly lower than, COMPLEX II estimates. CITPUFF (PPSP) results yield high near-source values, but lower values than COMPLEX II and CITPUFF (Pasquill-Gifford) at distances beyond the second mound.

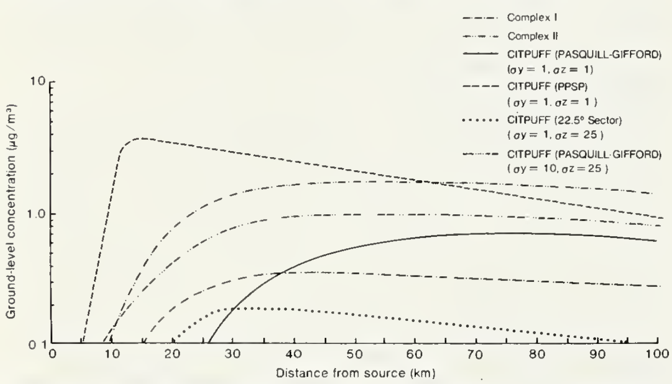

Figure 13.—Flat terrain comparison of COMPLEX I, COMPLEX II, and CITPUFF (plume height = 300 m, emissions = 100 g/s, wind—west at 4 m/s measured at 10 m, stability = E, CITPUFF runs vary by the definition of initial σ_y and σ_z at the source).

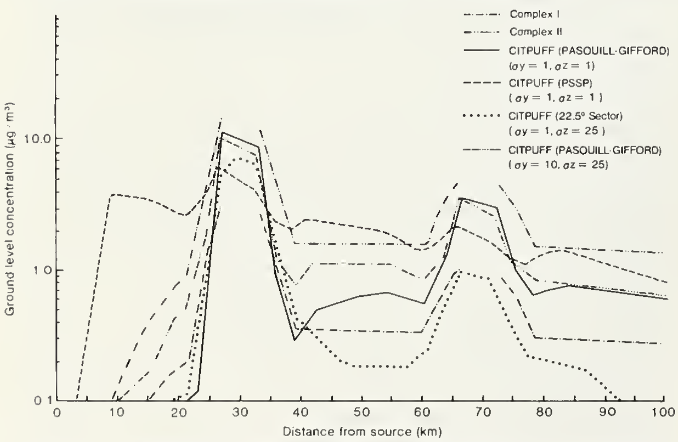

Figure 14.—Mounded terrain comparison of COMPLEX I, COMPLEX II, and CITPUFF (plume height = 300 m, emissions = 100 g/s, wind—west at 4 m/s measured at 10 m, stability = E, CITPUFF runs vary by the definition of initial σ_y and σ_z at the source).

The location of the highest ground-level concentration near the peaks occurs on the windward side of the peaks. When initial σ_y and σ_z values in CITPUFF are set to larger values to simulate area sources, the location of the highest concentrations could shift to the lee side of the peaks. These variations are due to the interaction of terrain, transport wind, and dispersion parameters.

Summary

COMPLEX I, COMPLEX II, and CITPUFF were compared over flat and idealized mounded terrain under stable conditions. Results were evaluated to a distance of 100 km from an elevated point source. Beyond 50 km in both terrain tests, all model results fell within the range of centerline ground-level concentrations defined by the low values estimated by CITPUFF (22.5° sector) and high values estimated by COMPLEX II. Results from a recent small-scale field experiment (Lavery et al. 1982) suggest that COMPLEX I ground-level values may be more realistic than COMPLEX II values. CITPUFF, depending on the selected dispersion option, estimated both higher and lower values than COMPLEX I and COMPLEX II.

Significant difficulties in the treatment of plume interactions with elevated terrain also will lead to differences with model results. The maximum value predicted by CITPUFF for elevated terrain is also quite sensitive to the assigned values of initial dispersion coefficients. The sensitivity of near-source ground-level concentrations due to initial dispersion coefficient values and due to variations among model concepts and applications are well known (EPA 1978).

Validation Requirements and Limitations on the Applications of CITPUFF

Dispersion formulations have been extensively evaluated, and the uncertainty associated with their use will probably never be less than a factor of two at best (Fox 1984, Fox et al. 1983). In fact, this is only under the most ideal of circumstances very close to the source. At distances beyond a few kilometers, recent model evaluations under such ideal circumstances (Londergan et al. 1982, Weber et al. 1982, Bowne et al. 1983) indicated that models showed little skill in predicting an observation at a particular time and location. Performance measures (Fox 1982) that reduce demands on the models indicate that the magnitude and frequency of occurrence of maximum values can be predicted with some skill.

In complex topography, air quality evaluations have tended to focus on the near-source problem, e.g., within a 2-5 km range. This is highlighted, for example, by the fact that the two data bases EPA currently recommends to evaluate complex topography models have no monitors farther than 5 km from the source. The CITPUFF model is not designed, and should not be used, for such a close-in impact analysis. At these distances, the puff approximation to the plume is questionable; the wind field

is not properly resolved and the puff centerline path correction factors would need to be evaluated with local data on Froude numbers.

All indications, however, suggest that at further distances from the source (say beyond 10 km) the puff dispersion within a wind field approach of CITPUFF is needed in complex topography (Egan 1984).[4] A comparison between CITPUFF, COMPLEX I, and COMPLEX II suggests that CITPUFF, applied using Pasquill-Gifford dispersion parameters, yields higher ground-level concentrations than COMPLEX I but lower values than COMPLEX II.

These factors combine to suggest that CITPUFF, in the absence of specific validation studies, can be expected to overpredict maximum ground-level concentrations. Because of this, it may be suitable for applications in environmental impact statements and for projecting worst case impacts in permit reviews. If applied to smoke management, it should provide a factor of safety by overpredicting likely impacts. Considerable experiences will be needed to determine if this factor of safety is too large or not. CITPUFF should be used with extreme caution for anything other than these worst case screening (EPA 1978) applications.

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APPENDIX 1

COMPARISON OF VARIOUS DISPERSION SCHEMES USED IN CITPUFF

Comparisons among PPSP and Pasquill-Gifford dispersion techniques as applied in CITPUFF were made for σ_y (stability classes A, C, and F) and σ_z (stability classes C and F). These results were also compared to the Turner Workbook nomograms. Sigma values were tested from 0 to 100 km distances from the source. Figures A1 through A3 present the σ_y comparisons for A, C, and F stabilities, respectively. Figures A4 and A5 present the σ_z comparisons for C and F stabilities.

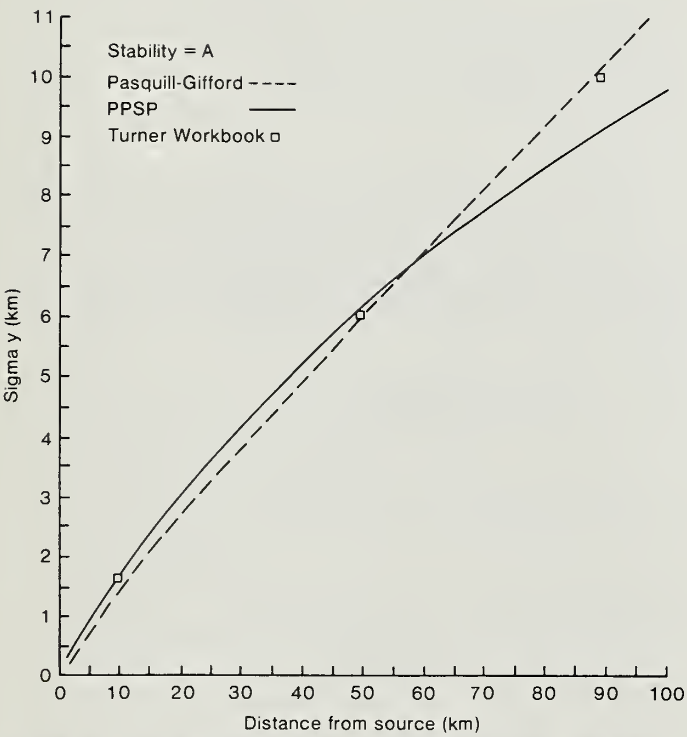

Figure A1.—PPSP, Pasquill, and Turner horizontal dispersion comparison (σ_y) for stability A.

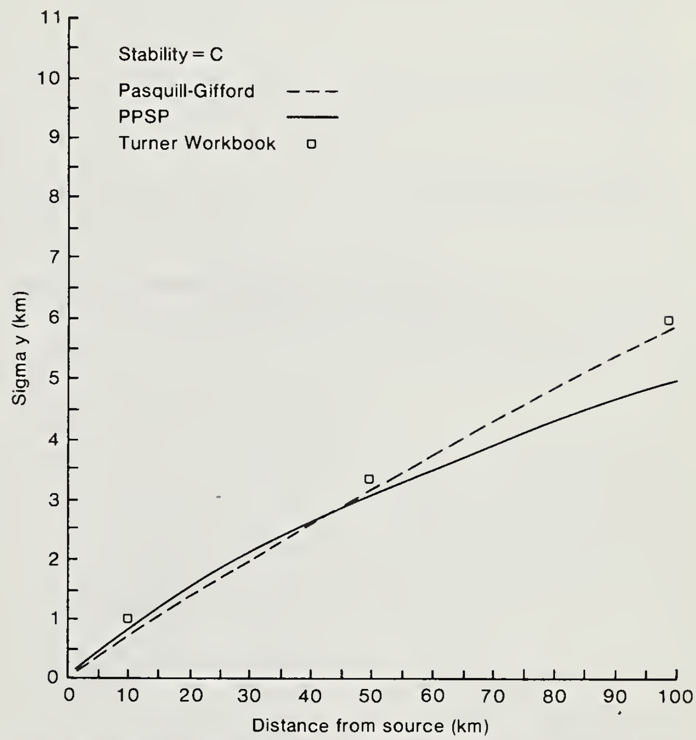

Figure A2.—PPSP, Pasquill, and Turner horizontal dispersion comparison (σ_y) for stability C.

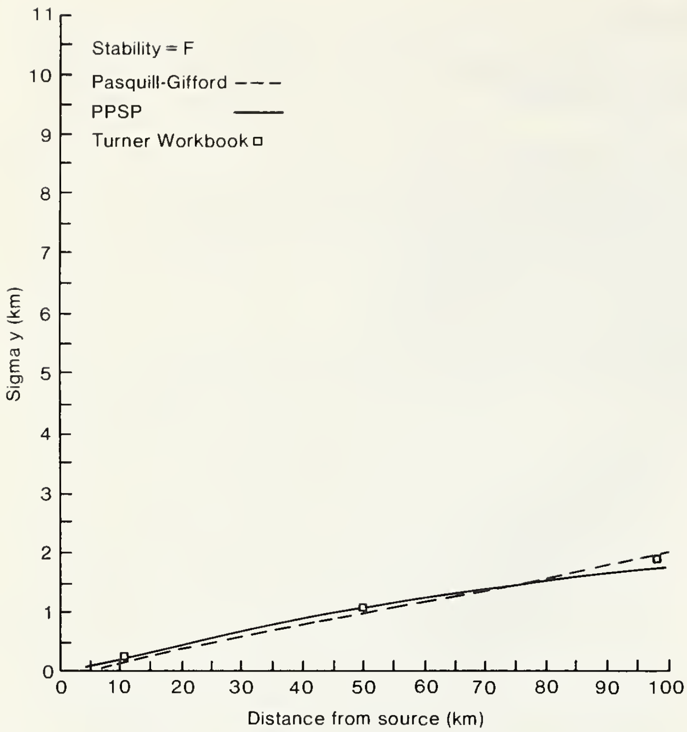

Figure A3.—PPSP, Pasquill, and Turner horizontal dispersion comparison (σ_y) for stability F.

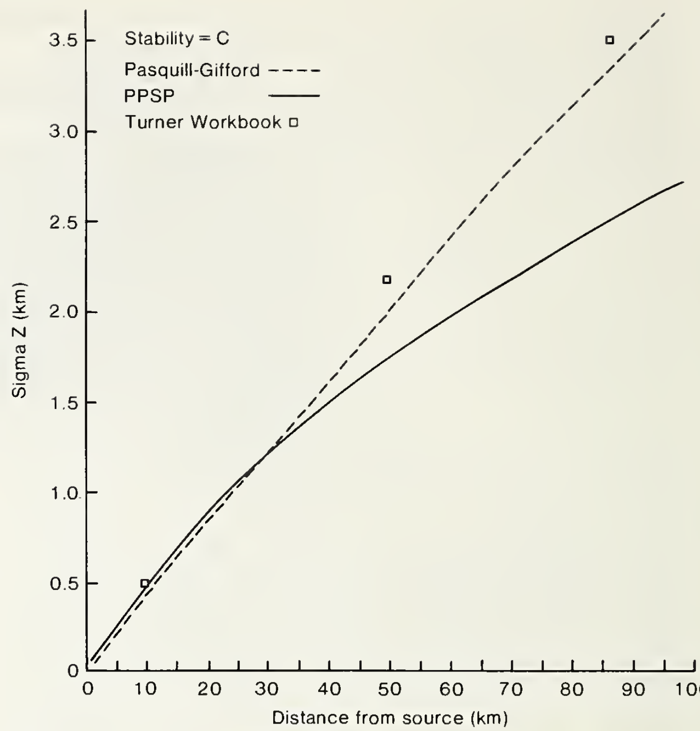

Figure A4.—PPSP, Pasquill, and Turner vertical dispersion comparison (σ_y) for stability C.

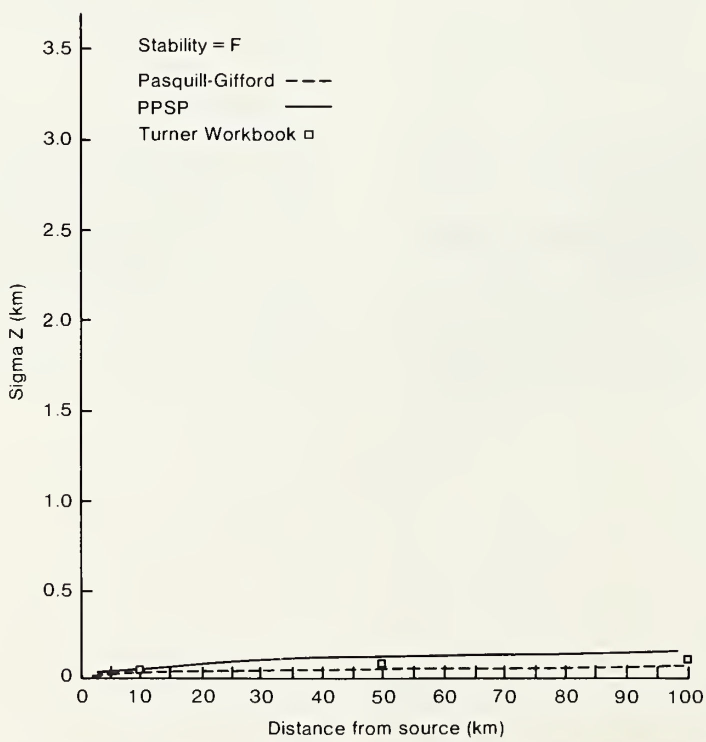

Figure A5.—PPSP, Pasquill, and Turner vertical dispersion comparison (σ_y) for stability F.

CITPUFF USER INSTRUCTIONS

CITPUFF has been implemented as part of the Topographic Air Resources Analysis System (TAPAS). TAPAS provides a modeling environment that supports the efficient application of CITPUFF. Results of other TAPAS models and data preparation routines such as the WINDS model and the Terrain Acquisition Routines can be used directly as input files to CITPUFF. In addition, the results of CITPUFF are generated in a TAPAS-structured file format that allows them to be directly accessed by TAPAS graphic plotting routines. TAPAS is currently implemented on the Colorado State University CDC Cyber 720 computer.

The CITPUFF package consists of a collection of programs, data, and procedure files that are designed to configure CITPUFF for various grid dimensions, set model boundary conditions, read data, and output results (Fox et al. 1984).

To run the CITPUFF package, the user must have the following files on the computer account:

- CITPUFF—Fortran code of the CITPUFF program
- PUFPROC—a multiple file of procedures to support CITPUFF configuration, input, run, and output routines
- TAPAS = structured files of u and v wind vector components of simulated wind field data to be used by CITPUFF in calculating puff trajectories
- A TAPAS-structured file of gridded terrain data for the desired analysis area
- A Control Parameter File—a file generated by the user to define the boundary conditions for CITPUFF modeling
- A Meteorological Data File—a file defining the date, time, mixing height, and ambient temperature for each hour of simulation
- USERNBR—a file containing the user's computer account number and password

Without these files the user will be unable to run the CITPUFF package.

Configuring CITPUFF for the Appropriate Grid Size

The computational arrays within CITPUFF must be configured for each analysis area. A procedure file has been developed to make the configuration of CITPUFF a simple operation. The configuration procedure (PUFCHNG) has the following form:

– PUFCHNG,PUFPROC,MEX,MEY,ICOLS,JROWS, REL,RUN,STEP,RATE = BKG,JOBID = DD77

Specifically, the user should type the following:

1. A dash
2. PUFCHNG (This specifies that the user wishes to execute the PUFCHNG procedure file, which directs the reconfiguration of CITPUFF)
3. PUFPROC (PUFPROC is the group of procedure files that contain PUFCHNG and other support routines necessary for running CITPUFF)
4. MEX (Number of grid points in the x direction of the u and v wind components and elevation data files)
5. MEY (Number of grid points in the y direction of the u and v wind components and elevation data files)
6. ICOLS (Number of grid points in the x direction of the CITPUFF computational grid; usually the same value as MEX)
7. JROWS (Number of grid points in the y direction of the CITPUFF computational grid; usually the same values as MEY)
8. REL (Number of hours of emission release from defined sources)
9. RUN (Number of sources)
10. STEP (Number of time steps in hours. This value must be at least equal to the number of hours of the simulation plus one.)
11. RATE = BKG (This space is reserved for the CSU Computer Center job priority processing rate.) The default rate is background (BKG); the user accepts the default by typing two commas (,,). If other rates are desired, the user must type:

PRIME	(Top priority—full price)
BKG	(30% discount)
3RD	(Overnight—40% discount)

12. JOBID = DD77 (The default JOBID is DD77, indicating that the hard copy output will be titled with DD77 followed by a computer-generated three-character code. The user can accept the default by typing two commas (,,) or input another JOBID.)

When the procedure execution instruction is properly typed on the interactive terminal, the user can execute the procedure by hitting the carriage return. A message, the system-defined JOBID, will appear on the screen; this identifies that the procedure was successfully submitted. The result of the PUFCHNG procedure will be a properly configured binary (object code) version of CITPUFF, which will appear on the user's account under the name PUFFOBJ.

Control Parameter File

The Control Parameter File is created by the user to direct the CITPUFF model. The CITPUFF Control

Parameter File contains 12 card image sections that identify specific CITPUFF dimensions, parameters, and options. An example control parameter file is provided in figure A6. Each card type section of the Control Parameter File is listed in table A1 and highlighted in figure A6.

```
Card
Type
 1      CITPUFF TEST DATA
 2      1.E-10
 3        1 25 0 7 1 10 2 1 400 1 0 10
 4       F F 06 12 18 24 24 24
 5       2.859000 3.706000 1 81 1 61
 6       1 81 1 61 1.0 1.0
 7       2 24 1 "PASQGIF" 3.0
 8      T
 8a      50. 29.00 27.50 1.0 1.0 5.5 383.0 4.0
         20. 28.75 30.50 1.0 1.0 30.0 325.0 10.0
         100. 63.
         100. 63.
         100. 63.
         100. 63.
         100. 63.
         100. 63.
         100. 63.
         100. 63.
         100. 63.
         100. 63.
         100. 63.
         100. 63.
 9       100. 63.
         100. 63.
         100. 63.
         100. 63.
         100. 63.
         100. 63.
         100. 63.
         100. 63.
         100. 63.
         100. 63.
         100. 63.
         100. 63.
10      T
10a     .5 .5 .5 .5 0.0 0.0
11      T
11a     .15 .20 .25 .30 .35 .40
12      3
        "COPWSW4", 1, 0
12a     "COPW4",1, 6
        "COPNW3",1, 18
```

Figure A6.—Example CITPUFF control parameter file.

Table A1.—Card sections for Control Parameter File.

Card type	Format	Parameter	Description
1	8A10	TITLE	User-selected title of CITPUFF model run
2	Free (real)	CHIMIN	Minimum significant concentration value (this determines puff radius) (suggested value = 1.0E-10)
3	Free (integer)	ITIME	Time in hours for start of release
	Free (integer)	NSTEPS	Total number of hourly steps for simulation (Set NSTEPS = NRELSE + 1 in current version)
	Free (integer)	NC	Decay rate constant for non-conservative puffs (NC = 0, s^{-1}, for conservative case)
	Free (integer)	MNST	Month in which release started
	Free (integer)	TDAY	Day in which release started
	Free (integer)	TAU	Puff release frequency; number of minutes between puffs
	Free (integer)	DT	Number of minutes between each puff sampling (used only when KVDT = 0)
	Free (integer)	NN1	Number of advection steps into first hour for release (NN1-1 for most cases)
	Free (integer)	LIMPUF	Maximum number of puffs carried before screening out no longer contributing puffs
	Free (integer)	KVDT	Allows number of minutes between puff sampling to be variable as determined by speed of puff and specified minimum travel distance between sampling of puffs. For KVDT-1;DT determined within program. KVDT = 0:DT is used as specified (suggested value = 1)
	Free (integer)	KFLSH	Dose and concentration array controller 1—initializes the dose and concentration array to zero after each print as defined by PTIME 0—allows the dose and concentration array to accumulate
	Free (integer)	NTADV	Number of minutes in basic advection step (suggested value = 10)
4	Free (logical)	PRTDOS	Print Dosage Flag. If set to True (T), dosage arrays will be printed for each source at each of the selected times (see PTIME). Suggested value (F). The total dosage at the end of the simulation will always be printed regardless of the selection of PRTDOS
	Free (logical)	PRTCON	Print Concentration Flag. If set to True (T), concentration array will be printed for each source at each of the selected times (see PTIME). Suggested value (F). The total concentration array at the end of the simulation will always be printed regardless of the selection of PRTCON
	Free (integer)	PTIME(I)	I = 1,6 hours between first six outputs of dose matrix and concentration array. PTIME(6) is the time between all subsequent printouts for a given simulation
5	Free (real)	DELX	Spacing in kilometers between grid points in x direction
	Free (real)	DELY	Spacing in kilometers between grid points in y direction
	Free (integer)	MSX	Column subscript for left boundary of concentration field
	Free (integer)	MFX	Column subscript for right boundary of concentration field
	Free (integer)	MSY	Row subscript for bottom boundary of concentration field
	Free (integer)	MFY	Row subscript for top boundary of concentration field
6	Free (integer)	MIX	As for MSX on card 5 but for wind velocity field
	Free (integer)	MEX	As for MFX on card 5 but for wind velocity field
	Free (integer)	MIY	As for MSY on card 5 but for wind velocity field
	Free (integer)	MEY	As for MFY on card 5 but for wind velocity field
	Free (real)	CONVX	Conversion factor between concentration field and velocity field grids (e.g., for CONVX = 2 grid spacing for concentration field is twice that for the velocity field)
	Free (real)	CONVY	As for CONVX, but can be specified independently
7	Free (integer)	NRUNS	Number of sources (maximum 50)
	Free (integer)	NRELSE	Total number of hours of effluent release
	Free (integer)	MNUM	Model number: MNUM = 1, Gaussian distribution in the vertical; MNUM = 2, uniform vertical concentration distribution (suggested value = 1)
	Character	SIGTYP	Parameter used to select the dispersion method to be applied: the value for SIGTYP must be enclosed by double quotations: "PASQGIF" - Pasquill-Gifford based dispersion in y and z "PPSP" - Power Plant Siting Program method "SECTOR" - 22.5° sector dispersion in y and Pasquill-Gifford in z (as applied in COMPLEX I model)

	Free (real)	TMSWTCH	Time in hours at which dispersion calculations will switch from distance- to time-based algorithm. If dispersion is to be calculated based on distance for the entire simulation or if the SECTOR dispersion option is selected, TIMSWTCH should be set equal to 999.9
8	Free (logical)	CALRISE	Plume rise calculation switch: T (true) Calculate plume rise within model based on stack parameters given on the source parameter cards (card type 8a)
			F (false) Plume rise will not be calculated. The final plume rise is assumed to be the term HS as given in the source parameter cards (card type 8a)
8a	Source Parameter Cards—One card per each source (1 through NRUNS). Note: The use of the parameters listed below depend on the selection of CALRISE (card type 8)		
	Free (integer)	HS(NRUNS)	Stack height in meters above ground level
	Free (real)	XSO(NRUNS)	X coordinate of source in concentration grid units
	Free (real)	YSO(NRUNS)	Y coordinates of source in concentration grid units
	Free (real)	SIGY1(NRUNS)	Initial cross-wind sigma in meters
	Free (real)	SIGZO(NRUNS)	Initial vertical sigma in meters Note: If the 22.5° sector dispersion option is selected, the initial SIGZO must be set as 1.0. Because of the use of the COMPLEX I method of calculating σ_z, an initial σ_z greater than 1.0 will not be recognized by the model. With the Pasquill-Gifford or PPSP options any initial σ_z is allowed
The following three values are only used if CALRISE = T			
	Free (real)	EXTVEL(NRUNS)	Stack gas exit velocity in meters per second
	Free (real)	EXTTMP(NRUNS)	Stack gas temperature in °K
	Free (real)	DIAM(NRUNS)	Stack diameter in meters
9	Free (real)	QX(1,NRELSE)	Emission rate in gas per second (real)for source number 1
		QX(NRUNS, NRELSE)	Emission rate in gas per second for number NRELSE
10	Free (logical)	NEWTER	Terrain adjustment factor (TER) switch:
			T (true) The user must enter new terrain adjustment factors on the next card for A-F stabilities (card type 10a)
			F (false) The default terrain adjustment factors will be used; .5, .5, .5, .5, .3, .3. If NEWTER = F, card type 10a must not be included in the control parameter deck
10a	Free (real)	TER	User-selected terrain adjustment factors for A-F stability (used only if NEWTER = T)
11	Free (logical)	NEWPOW	Wind power law adjustment factors (SNP) switch:
			T (true) The user wishes to select his own wind power law for each stability. The user must enter the new power law exponent on next card for A-F stabilities (card type 11a)
			F (false) The default power law exponents will be used for A-G stabilities; .15, .15, .20, .25, .40, .60. If NEWPOW = F card type 11a must not be included in the control parameter deck
11a	Free (real)	SNP	User-selected wind power law exponent for A-F stability (used only if NEWPOW = T)
12	Free (integer)	NUMFIL	The number of wind velocity fields that are to be read and used in the simulation
12a	Wind Velocity Field Cards—One card containing each of the following parameters must be included for each wind velocity field to be used during the simulation		
	Character	FILEAR (NUMFIL)	Name of the TAPAS-structured file that contains the velocity field u and v arrays required for a given simulation period.[1] File name must be surrounded by double quotations
	Free (integer)	LOCARY (NUMFIL)	Block location number of first velocity field component (u component) within the file FILEAR
	Free (integer)	TIMEAR (NUMFIL)	Time (from start of algorithm) at which velocity fields are to be used. TIMEAR(1) can be zero or one

[1]*A single run of the WINDS model produces a direct-access TAPAS-structured file containing arrays for elevations, potential temperature, divergence, u component of velocity, v component of velocity, etc. The u and v components are sequential so that LOCARY is set at the location of the u component.*

Meteorological Data File

The Meteorological Data File is created by the user to represent all meteorological boundary conditions except wind speed and direction for the simulation. The file contains the date of the simulation, the stability category, mixing depth, and ambient temperature. The file must be at least 24-hr long (contain 24 cards) even if a CITPUFF simulation is performed for less than 24 hr. A sample Meteorological Data File is provided in Figure A7. Table A2 gives the structure of the Meteorological Data File.

```
0701 5 4300 288
0701 5 4300 288
0701 5 4300 288
0701 4 4300 291
0701 4 4300 291
0701 4 4300 291
0701 4 4300 291
0701 4 4300 291
0701 4 4300 291
0701 4 4300 291
0701 5 4300 293
0701 5 4300 293
0701 4 4300 293
0701 4 4300 293
0701 4 4300 293
0701 5 4300 289
0701 5 4300 289
0701 5 4300 287
0701 5 4300 287
0701 5 4300 285
0701 5 4300 285
0701 5 4300 285
0701 5 4300 285
0701 5 4300 285
```

Figure A7.—Example CITPUFF meterological data file.

Table A2.—Structure of Meteorological Data File.

Card type	Format	Parameter	Description
1	Free (integer)	MET(I,1)	MMDD, the first two digits denote the month and the second two the day
(I cards - one card in 24-hr blocks)	Free (integer)	MET (I,2)	Single digit from 1 to 6 denoting stability class (1 unstable, 4 neutral, 6 stable)
	Free (integer)	MET(I,3)	Height of mixing depth above mean sea level in meters
	Free (integer)	MET(I,4)	Average ambient temperature of analysis area in °K (used only for plume rise calculations)

CITPUFF Model Run Procedure File

Once the CITPUFF model has been configured, the Control Parameter and Meteorological Data files have been constructed, and the needed WINDS model results and elevation data are present on the user's account, the CITPUFF model can be run. A procedure file has been developed to simplify the running of the model. The procedure file provides the interface between the user and

the CDC computer operating system. The run CITPUFF procedure (RUNPUFF) has the following form:

– RUNPUFF,PUFPROC,CONTROL,METDAT, ELEVDAT,CONCEN,PUFFLOC,RATE = BKG, JOBID = DD77,DEST = $ID = 00$.

Specifically, the user should type the following:

1. A dash

2. RUNPUFF (This specifies that the user wishes to execute the RUNPUFF procedure file that directs the execution of CITPUFF)

3. PUFPROC (PUFPROC is the group of procedure files that contains RUNPUFF and other support routines necessary for running CITPUFF)

The next five parameters are specific to the user account and the specific CITPUFF run. User account file names should be substituted for the names provided here.

4. CONTROL (The user must enter the file name of the desired control parameter file)

5. METDAT (The user must enter the file name of the desired meteorological data file)

6. ELEVDAT (The user must enter the file name of the TAPAS-structured file containing the elevation data (in meters) of every grid point in the analysis area)

7. CONCEN (The user must select a file name that will contain the output results of the ground-level pollutant concentrations calculated by CITPUFF)

8. PUFFLOC (The user must select a file name that will contain the coordinate locations and other puff identification information for each puff from each source)

9. RATE = BKG (This space is reserved for the CSU Computer Center job priority processing rate.) The default rate is background (BKG); the user accepts the default by typing two commas (,,). If other rates are desired, the user must type:

PRIME	(top priority—full price)
BKG	(30% discount)
3RD	(Overnight—40% discount)

10. JOBID = DD77 (The default JOBID is DD77, indicating that the hard copy output will be titled with DD77 followed by a computer-generated three-character code. The user can accept the default by typing two commas (,,) or input another JOBID)

11. DEST = $ID = 00$ (The default destination code for hard copy output is the main CSU Computer Center (ID = 00). Output can be routed to any CSU site or specially designated location. To accept the default the user will type two commas (,,). To direct the output to another site the user must input the proper code as provided by the CSU Computer Center. For example, to route all output to the RMFRES the user would enter $UN = AW$.

When the procedure execution instruction is properly typed on the interactive terminal, the user can execute the procedure by hitting the carriage return.

CITPUFF Results

A hard copy printout of all model results will be automatically directed to the user-selected destination. CITPUFF will also generate four new files on the user's account:

- PUFF DAY—This is a dayfile listing the important steps in the execution of the CITPUFF package and includes total operating time and cost related units. The dayfile will indicate if any errors occurred in the run.

- PUFFOUT—This is a duplicate computer file of the hard copy output. If a run error is indicated in PUFFDAY, the user should review PUFFOUT to diagnose where the error occurred relative to the input parameters.

- CONCEN—Will contain the concentration fields as output in the hardcopy printout from CITPUFF. CONCEN (actually the user-defined name for CONCEN) will be written to the user's account as a direct-access, multiblock, TAPAS-structured file. Each concentration field, as requested by the user, will exist as a separate file on the multiblock CONCEN file. A schematic of the structure of CONCEN is provided as figure A8. CONCEN can be used directly as input to TAPAS contour graphics packages. More often, CONCEN is used in conjunction with other CITPUFF runs as input to the CITPUFF Results Data Handling Package. For a further explanation of the use of this package, see the CITPUFF Results Data Handling Package User's Guide—A TAPAS User's Guide available from the Rocky Mountain Station.

- PUFFLOC—Will contain the coordinate location, puff distance, and puff size of every modeled source. PUFFLOC can be used as a direct input into the PUFFPLT graphics package which can provide a visual representation of the modeled plume. (See the TAPAS—User's Guide to the Puff Trajectory Graphics Package available from the Rocky Mountain Station.)

The Control Parameter File for this example (COPCON1) is listed in figure A9. The Meteorological Data file COPMET is similar to that shown in Figure A7 except that the temperatures were fixed at 293° for all 24 hours. Wind field u and v components for this analysis were contained within the TAPAS-structured file COPWSW4. The terrain data TAPAS-structured file was named COPELVC.

Ground-Level Concentration Summary Files (in $\mu g/m^3$)

	Ground-level concentration contribution from source 1 at PTIME(1)
	Ground-level concentration contribution from source 1 at PTIME(2)
Source 1	. . .
	Ground-level concentration contribution from source 1 at PTIME(6)
	Ground-level concentration contribution from source 2 at PTIME(1)
	Ground-level concentration contribution from source 2 at PTIME(2)
Source 2	. . .
	Ground-level concentration contribution from source 2 at PTIME(6)
. . .	. . .
	Ground-level concentration contribution from source n at PTIME(1)
	Ground-level concentration contribution from source n at PTIME(2)
Source n	. . .
	Ground-level concentration contribution from source n at PTIME(6)
All Sources for the entire simulation (NSTEPS)	Total ground-level concentration from all sources for the entire simulation (NSTEPS)

Figure A8.—Schematic of CITPUFF ground-level concentration results file (CONCERN).

```
PROTOTYPE OIL SHALE = CITPUFF TEST DATA
1.E-10
 1 13 0 7 1 10 2 1 400 1 0 10
 F F 12 12 12 12 12 12
 2.859000 3.706000 1 81 1 61
 1 81 1 61 1.0 1.0
 2 12 1 "PASQGIF" 3.0
F
300. 29.00 27.50 125. 75.
300. 28.75 30.50 125. 75.
 101. 67.
 101. 67.
 101. 67.
 101. 67.
 101. 67.
 101. 67.
 101. 67.
 101. 67.
 101. 67.
 101. 67.
 101. 67.
 101. 67.
F
F
1
"COPWSW4", 1, 0
```

Figure A9.—Control parameter file listing for the example CITPUFF analysis.

CITPUFF Configuration for the Example Analysis

The CITPUFF model configuration procedure instructions had the form

– PUFCHNG,PUFPROC,81,61,81,61,24,2,25

The configured binary version of the model was stored on the user account as PFFOBJ.

CITPUFF Example Run

The procedure instruction to run this example had the following form:

– RUNPUFF,PUFPROC,COPCON1,COPMET,
COPELVC,CONCEN1,PUFLOC1,,,,

The dayfile output from this 12-hr simulation is listed in figure A10.

```
11.30.48.DD77,T5000,PR200.
11.30.49.USER,CCC9AA4,.
11.30.50.ROUTE,OUTPUT,DEF,DC = LP,ID = 00.
11.30.51.  ROUTE  COMPLETE.
11.30.51.RATE,BKG.
11.30.51.SDAD,  0.001KUNS.
11.30.51.SDPF,  0.004KUNS.
11.30.51.SDMS,  0.143KUNS.
11.30.51.SDCP,  0.014SECS.
11.30.51.SDSR,  1.036UNTS.
11.30.51.  RATE COMPLETE.
11.30.51.GET,TAPE6 = COPCON1.
11.30.52.GET,TAPE5 = COPMET.
11.30.52.BEGIN,MAKLOC2,PUFPROC,COPELVC,TAPE8.
11.30.54.IFE,FILE(COPELVC,LO).OR.FILE(COPELVC,PT),LOCAL.
11.30.54.ENDIF,LOCAL.
11.30.54.GET,TAPE8 = COPELVC/NA.
11.30.56.IFE,FILE(TAPE8,LO),INDIR.
11.30.56.COMMENT.  *****  GET SUCCESSFUL. COPELVC NOW LOCAL AS TAPE8.
11.30.56.REVERT.MAKLOC
11.30.56.DEFINE,TAPE14 = CONCEN1,TAPE13 = PUFLOC1.
11.30.57.GET,PUFFOBJ.
11.30.58.PUFFOBJ.
11.35.57.  END CITPUFF
11.35.57.  173500 MAXIMUM EXECUTION FL.
11.35.57.  242.599 CP SECONDS EXECUTION TIME.
11.35.57.RETURN, TAPE5,TAPE6,TAPE8,PUFFOBJ,TAPE13,TAPE14.
11.35.58.REWIND,TAPE10.
11.35.58.SKIP,EXLAB.
11.35.58.ENDIF,EXLAB.
11.35.58.REPLACE,OUTPUT = PUFFOUT/NA.
11.35.59.STIME  295.667 UNTS.
11.35.59.CTIME  245.843 SECS.
11.35.59.DAYFILE,L = PUFFDAY.
```

Figure A10.—Listing of the dayfile PUFFDAY for this example CITPUFF analysis.

Ross, D. G., D. G. Fox, D. L. Dietrich, J. E. Childs, and W. E. Marlatt. 1985. CITPUFF: A Gaussian puff model for estimating pollultant concentration in complex terrain. USDA Forest Service Research Paper RM-261, 24 p. Rocky Mountain Forest and Range Experiment Station, Fort Collins, Colo.

CITPUFF is a puff-type dispersion model that uses a wind field calculated from a complex-terrain wind model. It accommodates a variety of source types including point, area, and line sources; calculates plume rise where applicable; and outputs a graphic display of puff trajectories and concentrations. The model is compared against models currently used for assessing air quality impacts in complex topography.

Keywords: Dispersion modeling, air pollution, mountain meteorology

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